Supporting Information

Fluoride Counterion Boosts Gold(I) Catalysis: Case Studies for Hydrodefluorination and CO_2 Hydrosilylation

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1. General experiment information

Chemicals and Solvents

Chemicals were purchased and used as received without further purification. Solvents were purified using a Mbraun SPS-800 Solvent Purification System. **LAuCl** was synthesized according to our previous report.[1]

Physical Measurements and Instrumentation

Gas chromatography/mass spectrometry (GC/MS) spectra were acquired on a 7890A GC system/5975C Mass spectrometer, while electrospray ionization mass spectrometry (ESI-MS) spectra were obtained on a Bruker APEX IV Fourier Transform Ion Cyclotron Resonance Mass Spectrometer. The crystal intensity data of **LAuHF$_2$** were collected on a Bruker Smart ApexII CCD diffractometer using graphite-monochromated Mo Kα radiation (0.71073 Å) at 296 K. High resolution mass spectrum (HR-MS) spectra were recorded on Bruker Solarix XR Fourier Transform Ion Cyclotron Resonance Mass Spectrometer using electrospray ionization. Mass spectrometric simulations were carried out using the IsoPro v3.0 package. Element analysis were recorded on a vario EL cube for C and H elements, and a Vario MICRO CUBE elemental analyzer of Elementar Analysensysteme GmbH for O element. Nuclear magnetic resonance (NMR) spectra including ^{1}H, ^{19}F, ^{13}C, and ^{31}P{H} were recorded on a Bruker 400 MHz instrument at 298 K. Chemical shifts were reported in ppm, and coupling constants were measured in Hz. The ^{1}H NMR spectra were referenced to residual protons, the ^{13}C NMR spectra were referenced relative to solvent resonances, the ^{31}P{H} NMR spectra were referenced to external 85% H_3PO_4 at δ 0 ppm, and the ^{19}F NMR spectra were referenced to external (CCl_3F, δ 0.0 ppm).

2. Experiment procedures

2.1 General produre for catalytic HDF reactions

In a glovebox, a 25 mL Schlenk tube containing **LAuHF$_2$** (1.5 mg, 0.002 mol), fluoroarenes (0.2 mmol), internal standard benzotrifluoride (3 μL), and 2 mL THF was prepared. An initial ^{19}F spectrum was recorded at room temperature, after which silanes (0.2 mmol) were added to the tube and the reaction was allowed to proceed for 2 hours in the dark. When the reaction was completed, a small portion of the reaction mixture (~0.2 mL) was taken from the Schlenk tube and passed through a short column of silica gel using CH_2Cl_2 as the eluent to obtain a sample for GC/MS analysis. Another 0.5 mL of the reaction mixture was directly transferred into an NMR tube for NMR analysis, and the yields of products were determined by integration in the ^{19}F NMR spectrum compared to the internal standard $PhCF_3$.

2.2 General produre for the formylation of amines using CO_2 and hydrosilanes

The catalyst **LAuHF$_2$** (1.5 mg, 0.002 mmol) was added to a two-necked flask equipped with a CO_2-filled balloon and a rubber septum. The flask was degassed by three freeze-pump-thaw cycles and then exposed to approximately 1 atmosphere of CO_2. Silane (0.2 mmol), amine (0.2 mmol), and 2-2.5 mL of anhydrous THF were added and stirred at room temperature for two hours. The resulting mixture was dissolved in 0.5 mL of $CDCl_3$ and characterized by ^{1}H NMR spectra. Yields were determined by ^{1}H NMR spectra of the crude reaction mixture using a specific amount of *p*-xylene as an internal standard. To isolate the products, the reaction mixture was diluted with ethyl acetate, and the resultant solution was concentrated and purified by silica gel column chromatography to obtain the corresponding formamides.

2.3 Synthesis of LAuHF$_2$

LAuCl (73.0 mg, 0.10 mmol) and one equivalent of $AgHF_2$ (14.6 mg, 0.10 mmol) were dissolved in anhydrous methanol in a Teflon flask and stirred at room temperature for 15 min. The reaction mixture was filtered through Celite and the filtrate was evaporated under vacuum. Then the crude product was recrystallized using a mixture of dichloromethane and diethyl ether. The final product was obtained as a white powder (45.4 mg, 62% yield). The **LAuHF$_2$** product was characterized by ^{1}H NMR (400 MHz, CD_3CN) with chemical shifts at δ 16.28 (t, J = 121.1 Hz, 1H), 7.64 (dd, J = 7.8, 1.4 Hz, 2H), 7.56 – 7.48 (m, 2H), 7.22 (t, J = 7.8 Hz, 2H), 1.40 (s, 6), and 1.31 – 1.14 (m, 36H). ^{31}P NMR (162 MHz, CD_3CN) had a chemical shift at δ 70.54, while the ^{19}F NMR (377 MHz, CD_3CN) had a chemical shift at δ -149.13 (d, J = 122.4 Hz). ^{13}C NMR (151 MHz, CD_3CN) δ 155.0, 135.9, 134.2, 130.0, 125.4, 125.4, 125.4, 117.3, 117.2, 38.3, 38.3, 38.2, 36.7, 30.5, 30.5, 30.5, 28.4. ESI-MS m/z: Calcd. For $C_{31}H_{48}AuOP_2$ (**LAu$^+$**) 695.2841, found 695.2826. Anal. Calcd for $C_{31}H_{51}O_2F_2P_2Au$ (**LAuHF$_2$**+H_2O): C, 49.47; H, 6.83; O, 4.25, found C, 48.63; H, 6.78; O, 4.25.

3. Electrochemistry

All electrochemical experiments were conducted using a standard three-electrode configuration on a Shanghai Chenhua CHI660C electrochemical workstation at room temperature (25 ºC) under argon or CO_2 atmospheres. Cyclic voltammetry experiments were recorded using glassy carbon working electrode disks with a diameter of 3 mm (Cypress Systems EE040). The working electrode was treated between scans by polishing with diamond paste (Buehler) of decreasing sizes (3 to 0.05 μm) interspersed with washing with purified H_2O. The auxiliary electrode was a platinum wire electrode, and an Ag/AgCl electrode was used as the reference electrode. All glassware for electrochemical experiments was oven-dried overnight and allowed to cool to room temperature before use.

Controlled-potential electrolysis (CPE) experiments were carried out using a 2 mM solution of the catalyst in 8 mL of 0.1 M nBu_4NPF_6 as electrolyte in dry DMF. A concentration of 5 M trifluoroethanol was added to the solution. The experiment was performed in a gas-tight

cell, and the electrolysis solution was purged with CO_2 for 20 minutes prior to electrolysis. A cyclic voltammetry (CV) scan was performed to establish the benchmark CPE potential. During electrolysis, the gases produced in the headspace were analyzed using a Shimadzu GC-2014 gas chromatography system equipped with two thermal conductivity detectors (TCD) for H_2 and CO detection, and a flame ionization detector (FID) for CH_4 detection. The flow rate of CO_2 was controlled at the inlet of the electrochemical cell using a standard series mass flow controller and measured by a flow meter at the exit of the electrochemical cell. However, no CO, H_2 CH_4 or other gas products were observed. The liquid products of electroreduction were analyzed by ^{1}H NMR spectrometry. The liquid phase was acidified with an aqueous solution of HCl (18%), spiked with a *p*-xylene internal standard, and then diluted with DMF-d7.

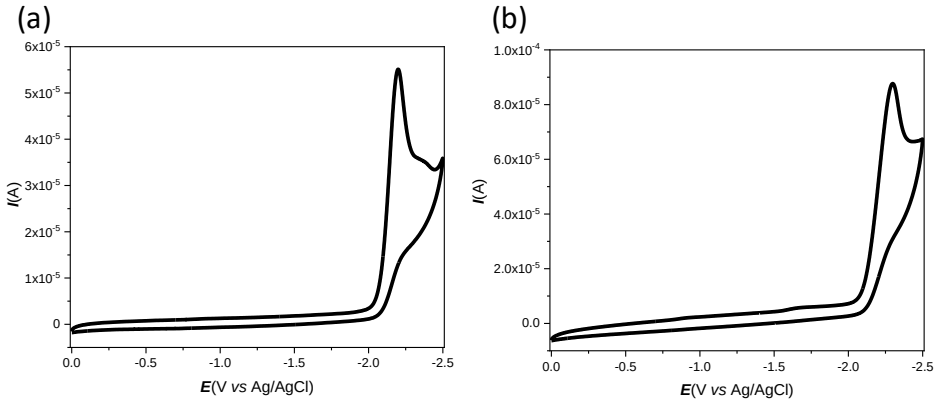


Figure S1. Cyclic voltammograms of complexes of 1.0 mM (a) **LAuHF$_2$** and (b) **LAuCl** with 0.1 M *n*But$_4$NPF$_6$ as electrolyte in dry DMF at 100 mV/s scan rate under Ar.

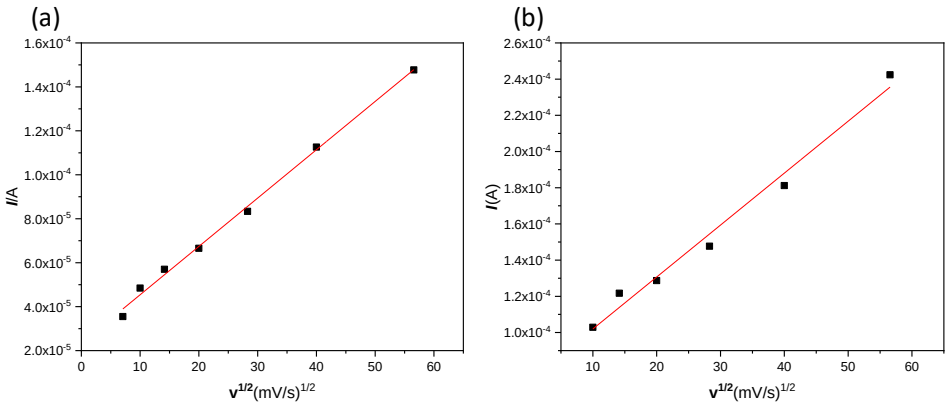


Figure S2. Plot of i_{cat} (A) vs. scan rate$^{1/2}$ (mV/s)$^{1/2}$ for (a) **LAuHF$_2$** and (b) **LAuCl**.

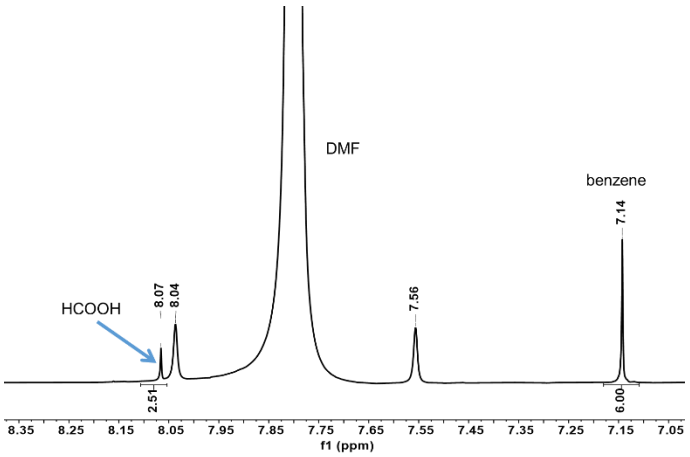


Figure S3. Liquid product of electrocatalytic CO_2 reduction through ^1H NMR characterization in DMF-d7.

4. Details for electrocatalytic turnover frequency (TOF) calculation

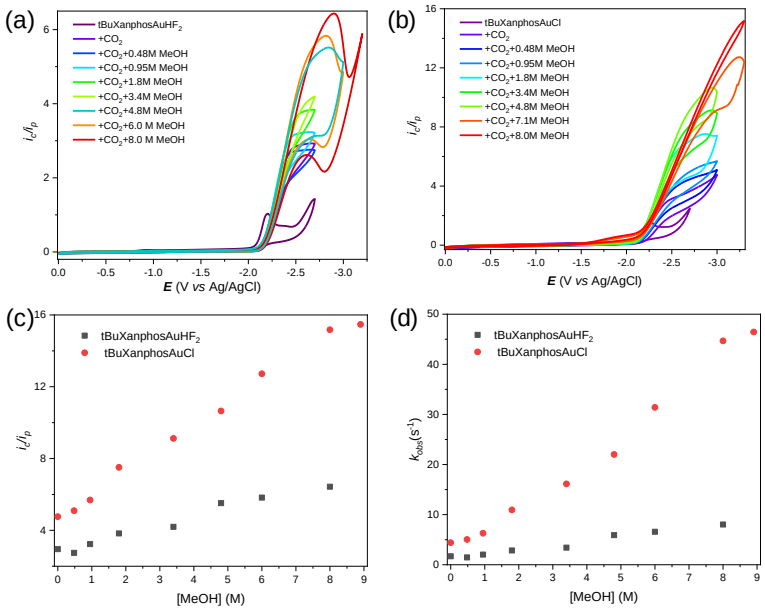


Figure S4. Successive cyclic voltammograms of 0.5 mM (a) **LAuHF$_2$** and (b) **LAuCl** in DMF (0.10 M nBu$_4$NPF$_6$ as electrolyte) at increasing concentrations of methanol. Conditions: 3 mm glassy-carbon working electrode; 25 °C; scan rate 100 mV/s. (c) Plot of i_c/i_p vs. concentration of methanol. (d) Plot of k_{obs} vs. concentration of methanol.

$$i_{cat} = n_{cat} FA[cat]\sqrt{Dk_{cat}[Q]^{y}} \qquad (1)$$

$$i_p = 0.4463 n_p^{\frac{3}{2}} FA[cat]\sqrt{\frac{FvD}{RT}} \qquad (2)$$

$$TOF = \mathrm{k_{cat}}[Q] = \frac{Fvn_p^3}{RT}\left(\frac{0.4463}{n_{cat}}\right)^2\left(\frac{i_{cat}}{i_p}\right)^2 \qquad (3)$$

TOF can be determined according to above 3 equations:

$$TOF = 1.94\mathrm{V}^{-1} v\left(\frac{i_{cat}}{i_p}\right)^2 \qquad (4)$$

Equations (1)–(3) were utilized to determine the turnover frequency (TOF) from catalytic cyclic voltammograms (CVs) using equation (4). Equation (1) provides the catalytic current peak (i_{cat}) and assumes pseudo-first-order kinetics, where the reaction is first order in catalyst and the substrate concentrations (Q) are much higher than that of the catalyst. In equation (1), n_{cat} represents the number of electrons needed for the catalytic reaction, while F is Faraday's constant (F = 96 485 C/mol). A denotes the electrode surface area (A = 0.07065 cm^2 for CVs), [cat] is the catalyst concentration ([cat] = 0.5 mM = 5×10^{-7} mol/mL), D is the diffusion constant of the catalytically-active species (~5×10^{-6} cm^2/s), k_{cat} is the rate constant of the catalytic reaction, and [Q] is the substrate concentration. The concentration of [CO_2] in dry DMF is 0.23 M (= 0.23×10^{-3} mol/mL), as previously reported.[2, 3]

Equation (2) includes R, the universal gas constant (R = 8.31 J K^{-1} mol–1), T, the temperature (T = 298.15 K), n_p, the number of electrons in the reversible non-catalytic reaction (n_p = 1 for the Au complexes system), and v, the scan rate (v = 0.1 V/s). By dividing equation (1) by equation (2), we can determine i_{cat}/i_p, which enables the calculation of the catalytic rate constant (k_{cat}) and TOF using equation (3). In equation (3), the surface area (A) cancels out because the same electrode was used for experiments under CO_2 and N_2. Additionally, D cancels out under the assumption that the diffusion constant of the catalytically active species remains constant under CO_2 and N_2. The peak i_{cat}/i_p and TOF values for the Au complexes can be calculated using equations (1)–(3), with i_p determined as the peak current under N_2.

5. Computation details

All calculations presented in this study were performed using the Gaussian 09 package.[4] The stationary points were geometry optimized using the B3LYP[5] hybrid functional with the 6-31G** basis set[6, 7] for main group atoms and the SDD pseudopotential with an associated basis set for gold, unless otherwise specified. Vibrational frequency calculations were performed at the same level of theory to confirm that each stationary point was either a minimum or a transition state. Single point energies and frequency calculations were computed using the B3LYP functional with "D3BJ"[8] dispersion corrections and the all-electron basis set of def2-TZVP[9]. Solvent effects were included using the SMD[10] model for tetrahydrofuran to match the experimental conditions. Transition states were characterized by a frequency calculation that resulted in a single imaginary mode for the proton transfer motion, and intrinsic reaction coordinate (IRC)[11] paths were calculated to connect each transition state to its corresponding reactant and product. The structures of intermediates and transition states were visualized using VMD 1.9.3.[12]

6. Summary of crystallographic data

Table S1. Crystal data and structure refinement

Complex	**$LAuHF_2$**
molecular formula	$C_{32}H_{51}AuCl_2FO_{1.5}P_2$
formula wt. (g mol^{-1})	808.53
temperature (K)	180.00(10)
radiation (λ, Å)	0.71073
crystal system	triclinic
space group	*P*-1
a (Å)	11.4363(3)
b (Å)	12.6303(3)
c (Å)	15.7917(4)
α (°)	67.371(2)
β (°)	73.525(2)
γ (°)	69.303(2)
Volume ($Å^3$)	1940.54(8)
Z	2
ρ_{calcd} (g cm^{-3})	1.384
μ (mm^{-1})	4.038
F(000)	814
crystal size (mm^3)	0.20×0.18× 0.15
Theta range	3.30 to 28.13°
reflections collected	28450
independent reflections	6823 [R(int) = 0.0439]
Completeness	99.8 %
goodness-of-fit on F^2	1.100
final R indices	$R1^a$ = 0.0447
[R > 2σ (I)]	wR_2^b = 0.1214
R indices (all data)	$R1^a$ = 0.0486 wR_2^b = 0.1243
largest diff. peak and hole (e $Å^{-3}$)	3.496 and -0.709

7. Supporting figures and tables

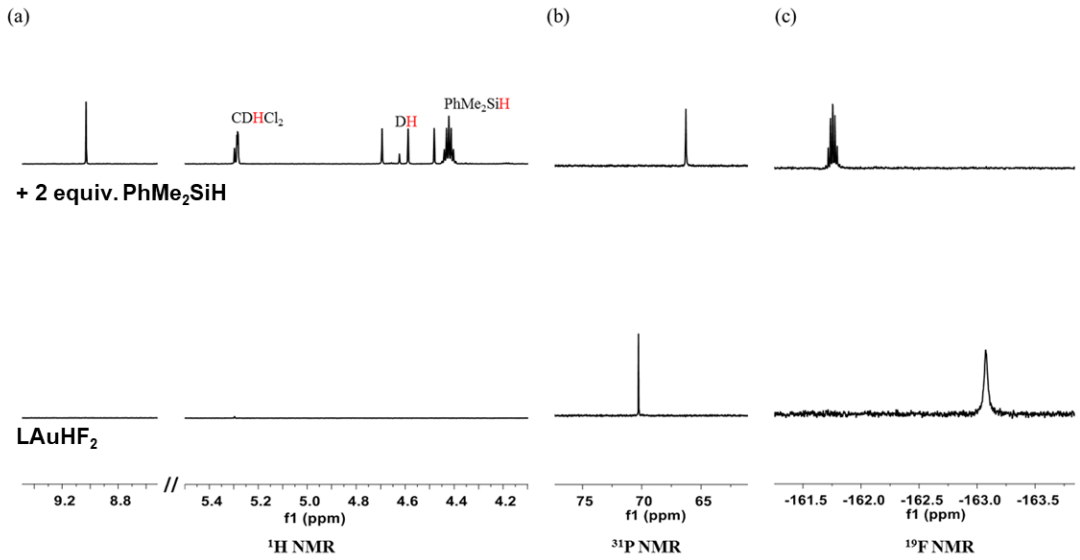


Figure S5. Stacked plot of (a) ^{1}H NMR, (b) ^{31}P{H} NMR and (c) ^{19}F NMR spectra of **LAuHF$_2$** titration with PhMe$_2$SiH in CDCl$_3$. The proton signal of ligand and solvent residue were omitted for clarification.

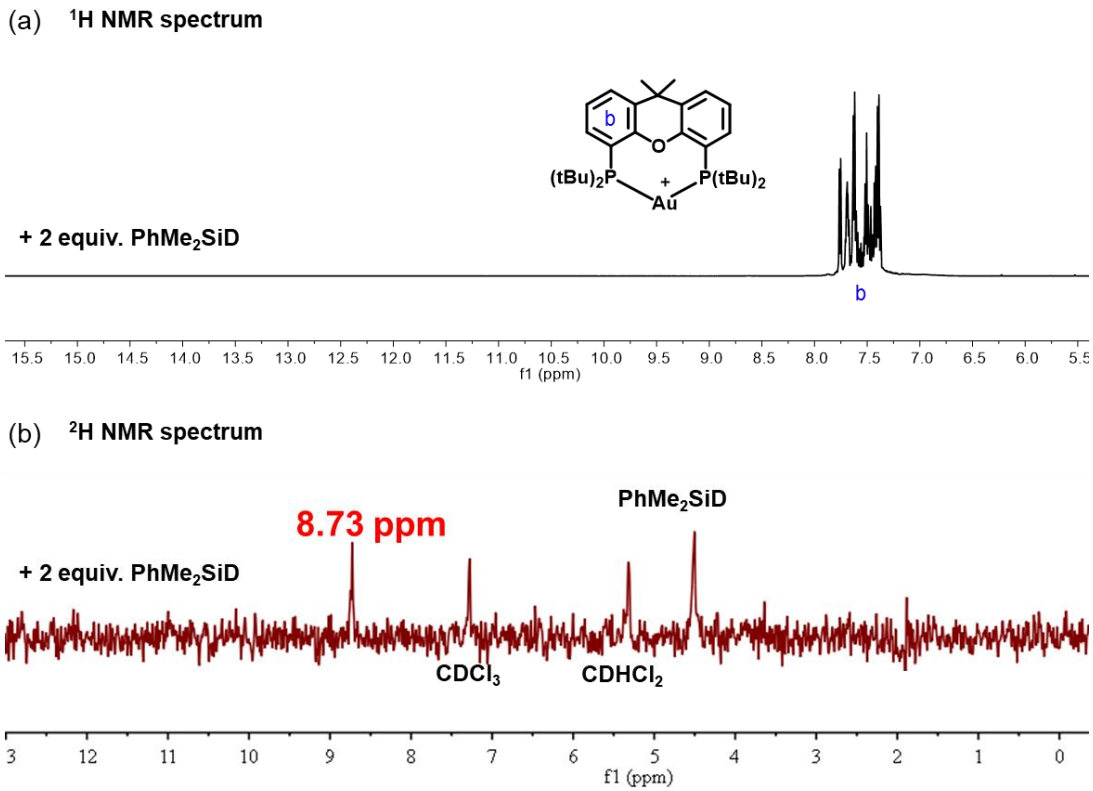


Figure S6. (a) ^{1}H NMR and (b) ^{2}H NMR spectra of **LAuHF$_2$** titration with 2 equiv. PhMe$_2$SiD in CDCl$_3$.

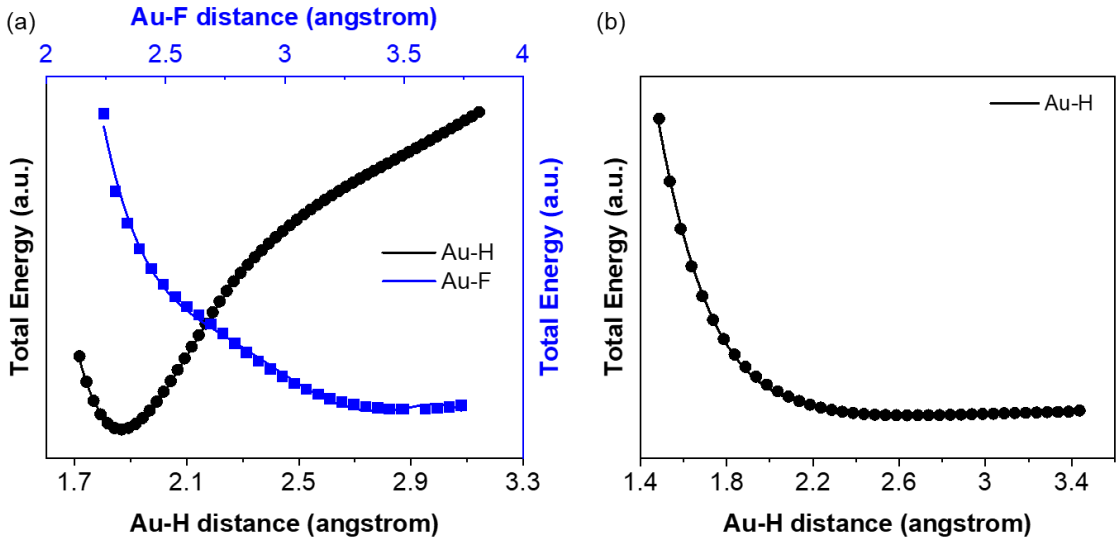


Figure S7. Relaxed surface scan of (a) Au-H and Au-F bonds in **LAuHF$_2$**, and (b) Au-H bond in **LAuCl** added with Ph_2SiH_2.

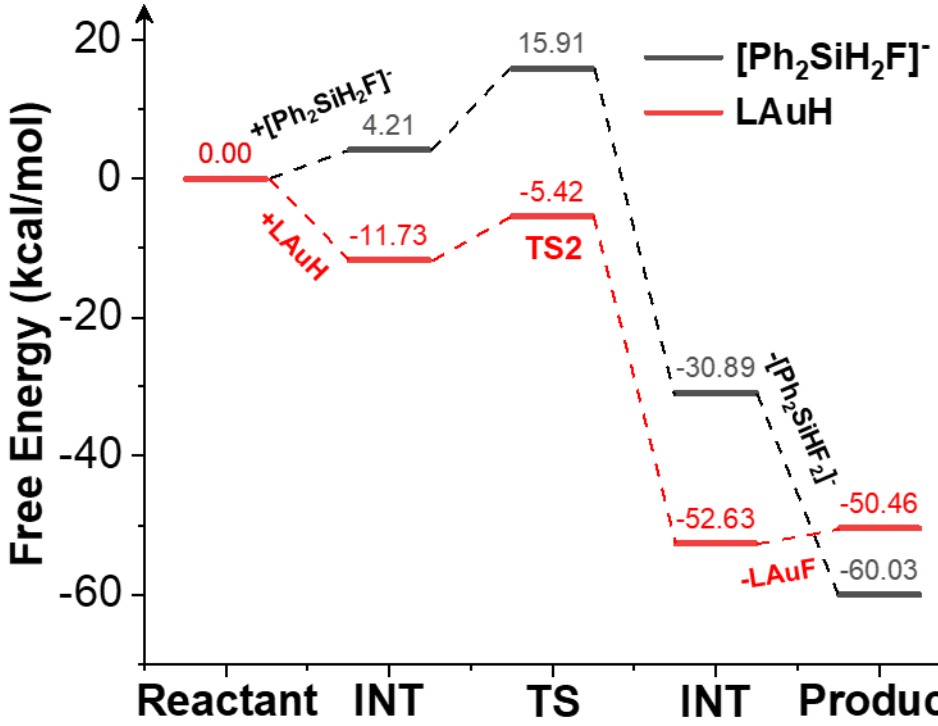


Figure S8. Computed free energy surface in HDF reaction for **[Au-H]** intermediate and fluorinion activated pentacoordinated silane.

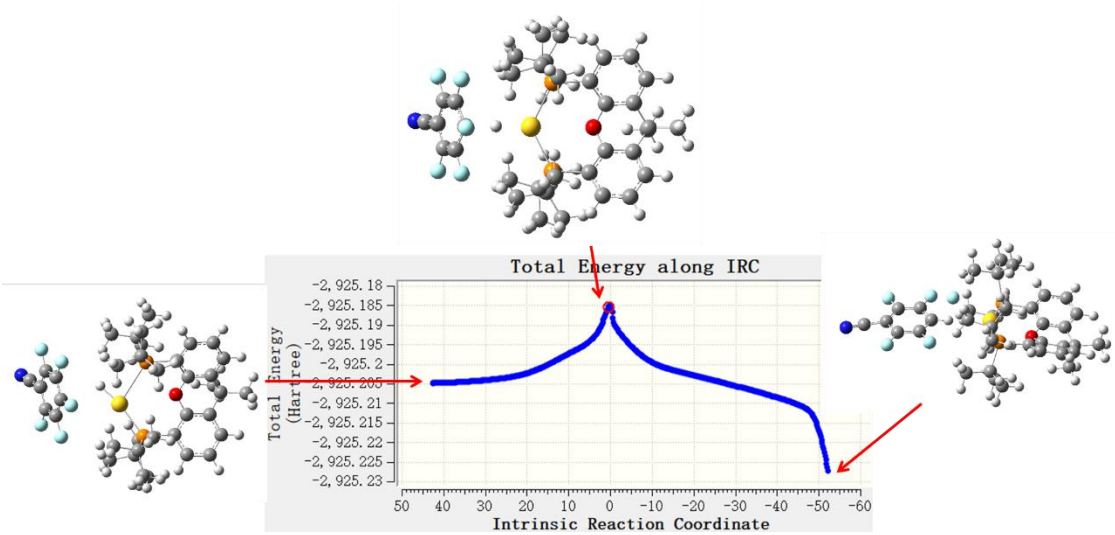


Figure S9. Calculated IRC path for HDF reaction catalyzed by **[Au-H]** intermediate in singlet spin state, connecting the transition state to the corresponding reactant and product.

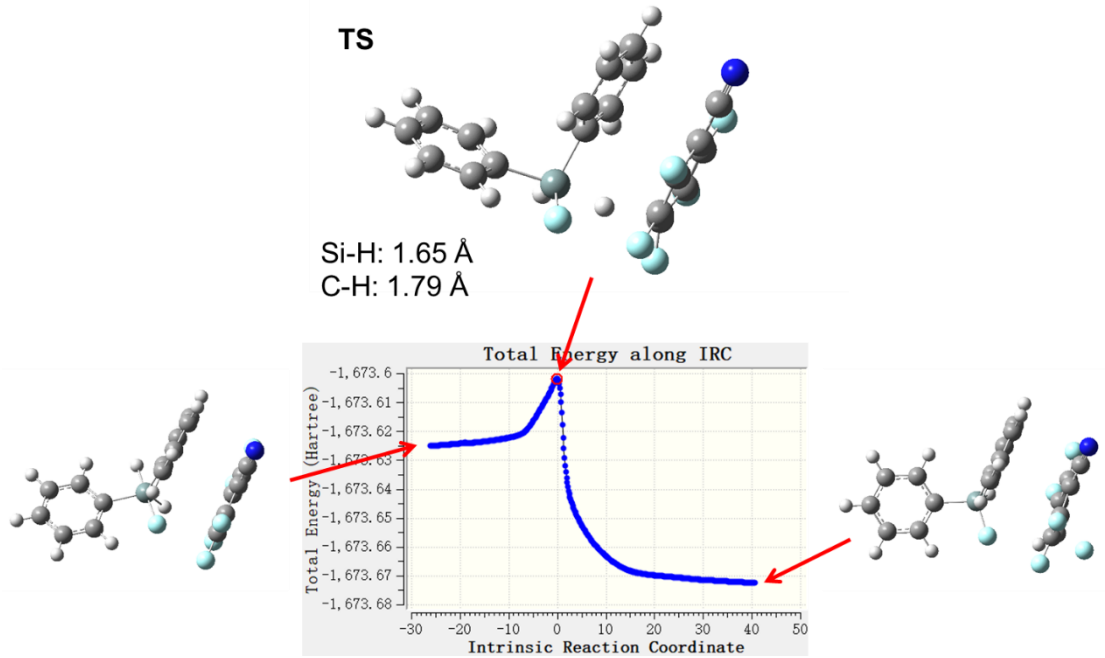


Figure S10. Calculated IRC path for HDF reaction catalyzed by $[Ph_2SiH_2F]^-$ in singlet spin state, connecting the transition state to the corresponding reactant and product.

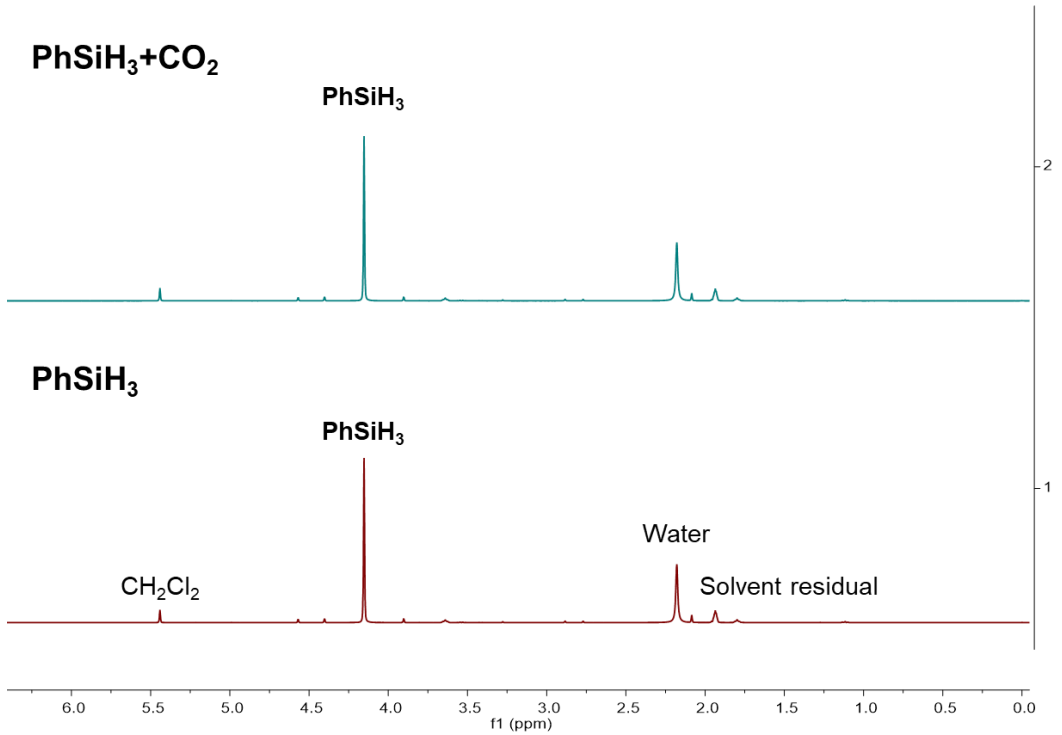


Figure S11. Stacked plot of ^{1}H NMR spectra of phenylsilane and CO_2 pumped into phenylsilane solution without in CD_3CN.

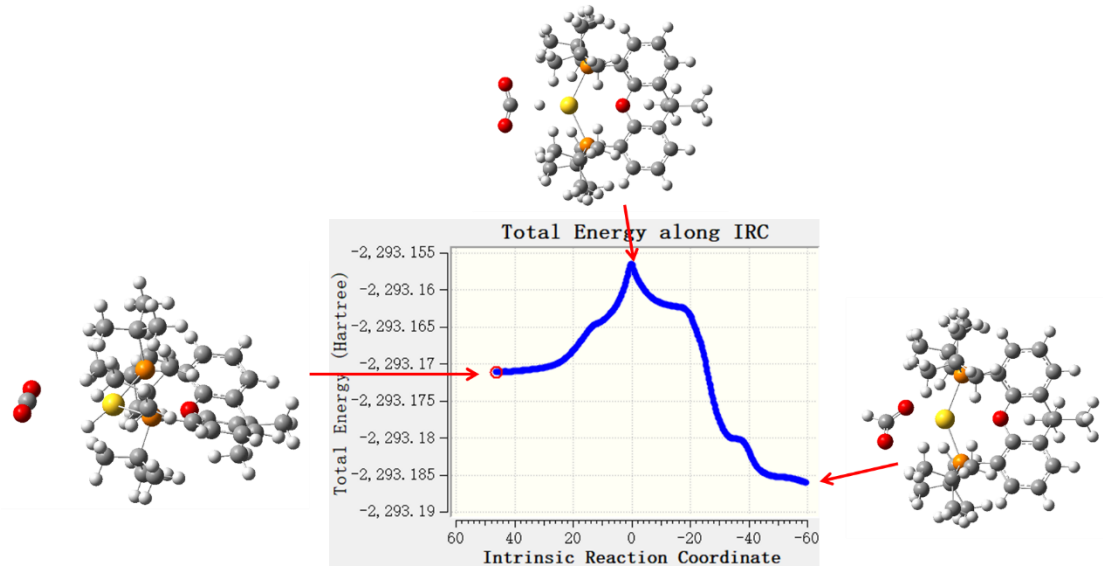
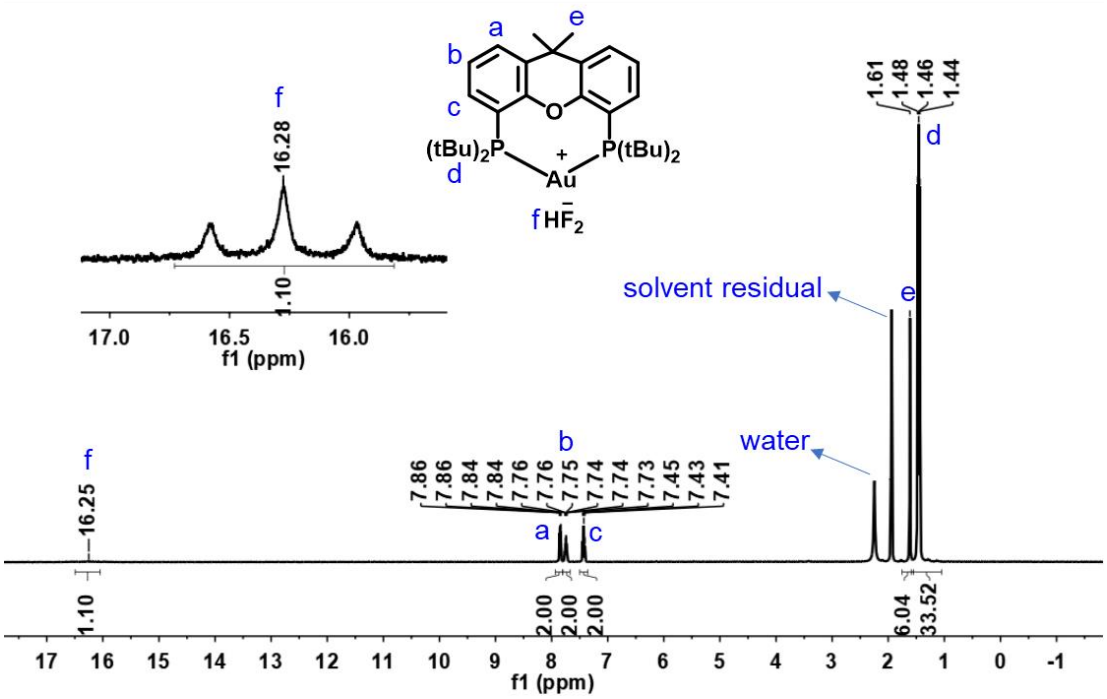
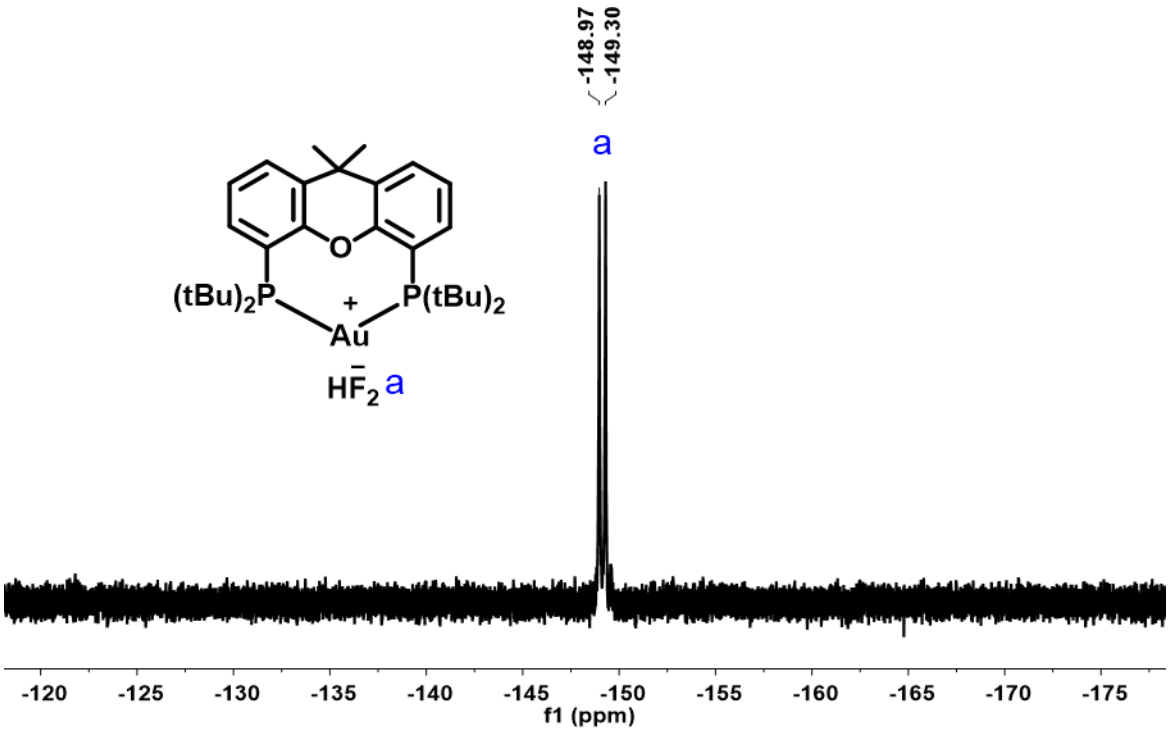


Figure S12. Calculated IRC path for CO_2 activation by **[Au-H]** intermediate in singlet spin state, connecting the transition state to the corresponding reactant and product.



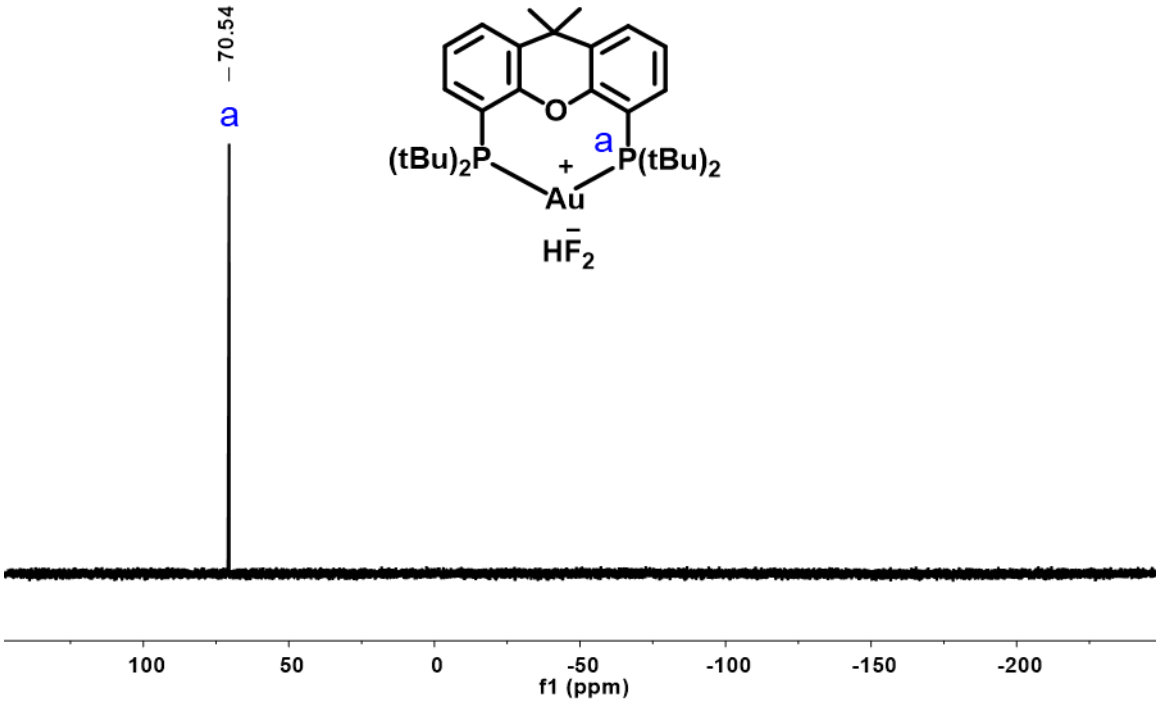
^{1}H NMR (400 MHz, CD_3CN) δ 16.28 (t, J = 121.1 Hz, 1H), 7.64 (dd, J = 7.8, 1.4 Hz, 2H), 7.56 – 7.48 (m, 2H), 7.22 (t, J = 7.8 Hz, 2H), 1.40 (s, 6), 1.31 – 1.14 (m, 36H).

Figure S13. ^{1}H NMR (400 MHz, CD_3CN solvent, 298 K) spectrum of **LAuHF$_2$**.



^{19}F NMR (377 MHz, CD_3CN) δ -149.13 (d, J = 122.4 Hz).

Figure S14. ^{19}F NMR (377 MHz, CD_3CN solvent, 298 K) spectrum of **LAuHF$_2$**.



^{31}P NMR (162 MHz, CD_3CN) δ 70.54.

Figure S15. ^{31}P{H} NMR (162 MHz, CD_3CN solvent, 298 K) spectrum of **LAuHF$_2$**.

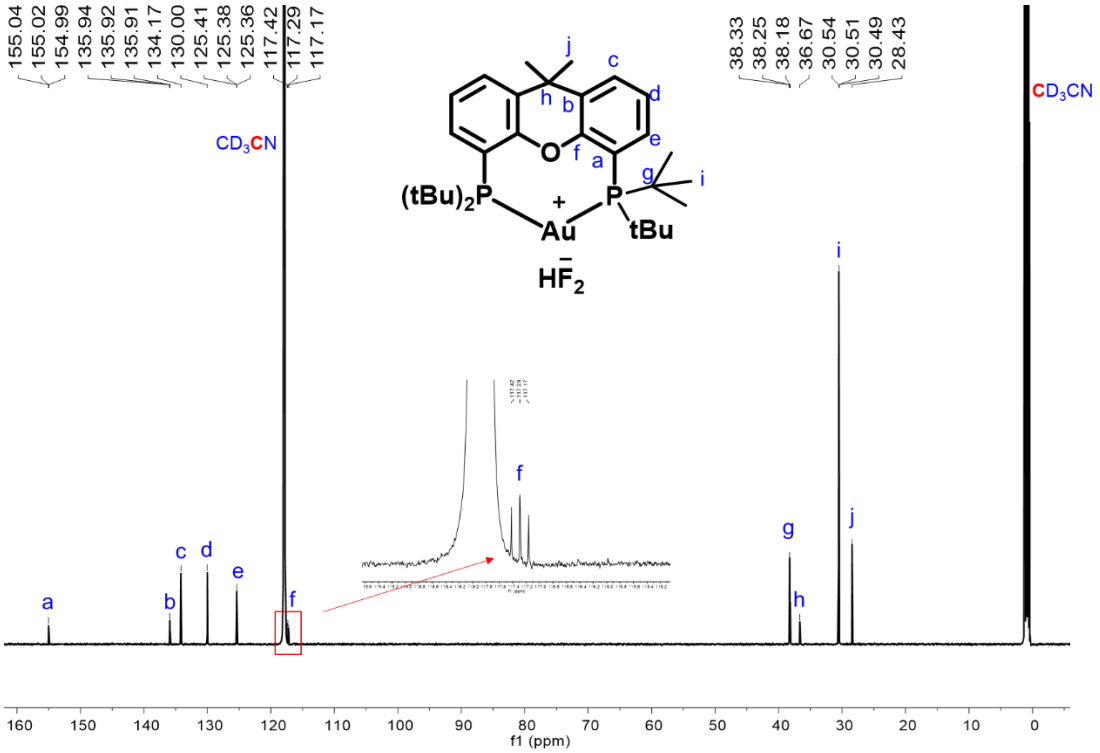


Figure S16. ^{13}C NMR (151 MHz, CD_3CN solvent, 298 K) spectrum of **LAuHF$_2$**.

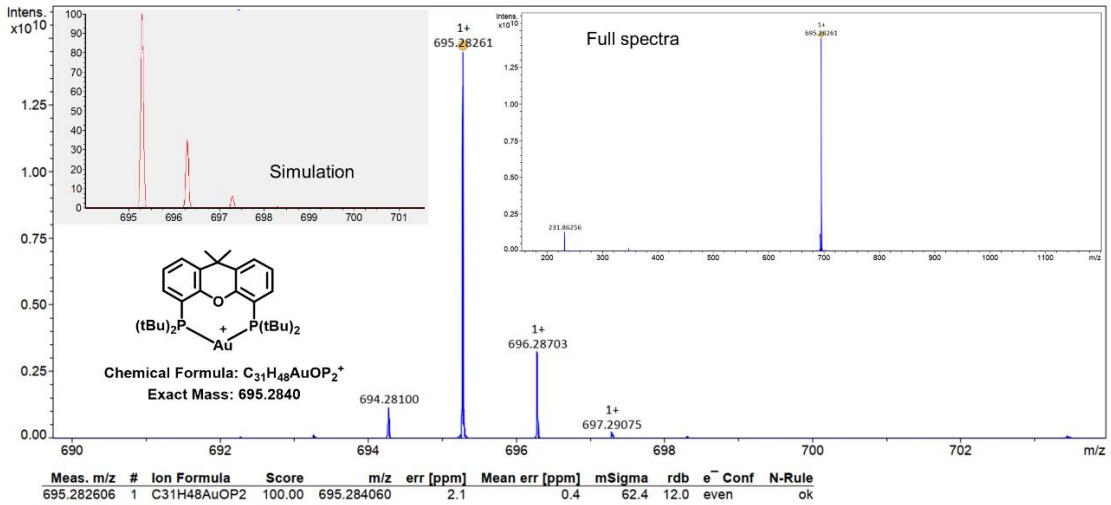
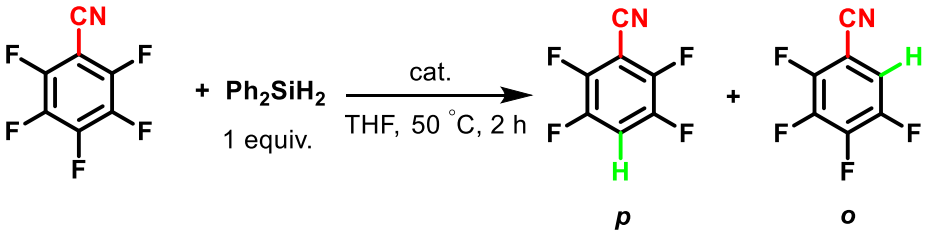


Figure S17. HR-MS (ESI-MS) of **LAuHF$_2$**. The insert shows the simulated isotopic pattern of the signal 695.2826 (m/z = 695.2826) and the full spectra.

Table S2. Reaction conditions optimization for fluorinion catalyzed HDF. [a]



Entry	Catalyst	R_3SiH	Yield (p/o, %)
1	LiF	Ph_2SiH_2	NR [c]
2	NaF	Ph_2SiH_2	NR [c]
3	KF	Ph_2SiH_2	NR [c]
4	CsF	Ph_2SiH_2	58/10
5 [b]	CsF	Ph_2SiH_2	85/10

[a] General reaction conditions: 0.2 mmol substrate, 10 mol catalyst, 50 °C, THF, 2h. [b] 10 mol% [18]-crown-6 was added as additive. [c] No reaction.

8. Product characterization

2,3,5,6-tetrafluorobenzonitrile (*p*-2a). ^{19}F NMR (471 MHz, THF-d_8) δ -135.12 – -135.30 (m, 2F), -137.64 – -137.79 (m, 2F).[1, 13]

2,3,4,5-tetrafluorobenzonitrile (*o*-2a). ^{19}F NMR (471 MHz, THF-d_8) δ -133.68 (ddt, *J* = 19.2, 12.5, 6.5 Hz, 1F), -137.87 (dtd, *J* = 21.4, 10.7, 4.0 Hz, 1F), -147.74 (tt, *J* = 20.5, 7.9 Hz, 1F), -154.66 – -154.83 (m, 1F).[1, 13]

2,3,5,6-tetrafluoronitrobenzene (*p*-2b). ^{19}F NMR (282 MHz, THF) δ -136.54 (d, *J* = 9.8 Hz, 2F) – -148..28 (t, *J* = 40.8 Hz, 2F).[1, 13]

2,3,4,5-tetrafluoronitrobenzene (*o*-2b). ^{19}F NMR (282 MHz, THF) δ -137.15 (d, *J* = 9.8 Hz, 1F), -143.21 (d, *J* = 40 Hz, 1F), -145.56 (t, *J* = 32.7 Hz, 1F), -152.19 (s, 1F).[13]

1,2,4,5-tetrafluoro-3-(trifluoromethyl)benzene (2c). ^{19}F NMR (282 MHz, THF) δ -57.10 (t, *J* = 22.1 Hz, 3F), -137.87 (dt, *J* = 19.7, 10.1 Hz, 2F), -142.20 (qtd, *J* = 23.7, 16.7, 15.8, 8.0 Hz, 2F).[1, 13]

Ethyl- 2,3,5,6-tetrafluorobenzoate (*p*-2d). ^{19}F NMR (471 MHz, THF) δ -134.92 (dh, *J* = 15.1, 8.1, 7.3 Hz, 2F), -137.34 – -137.52 (m, 2F).[14]

Pentafluorobenzene (2e/2g). ^{19}F NMR (282 MHz, THF) δ -139.66 (dt, *J* = 19.8, 8.9 Hz, 2F), -155.78 (d, *J* = 39.5 Hz, 1F), -163.62 (td, *J* = 20.6, 7.2 Hz, 2F).[15]

3-chloro-1,2,4,5-tetrafluorobenzene (*p*-2f). ^{19}F NMR (282 MHz, THF) δ -138.74 (p, *J* = 9.1, 8.6 Hz, 2F), -142.32 (dq, *J* = 20.1, 7.2, 6.2 Hz, 2F).[14]

2,3,5,6-tetrafluorobenzene (2h). ^{19}F NMR (282 MHz, THF) δ -140.27 (t, *J* = 8.7 Hz, 4F).[13]

2,3,6-Trifluoronitrobenzene (*p*-2i).^{19}F NMR (282 MHz, THF) δ -118.26 (ddd, *J* = 16.5, 13.7, 8.9 Hz, 1F), -124.21 (dq, *J* = 18.9, 9.2 Hz, 1F), -140.14 (ddt, *J* = 26.3, 15.6, 8.2 Hz, 1F).[16]

2,6-difluoronitrobenzene (*p*-2j). ^{19}F NMR (282 MHz, THF) δ -104.16 (dh, *J* = 7.7, 4.0 Hz, 2F).[16]

2,4-difluoronitrobenzene (*o*-2j). ^{19}F NMR (282 MHz, THF) δ -100.08 (dq, *J* = 13.8, 6.9 Hz, 1F), -113.08 (q, *J* = 11.2 Hz, 1F).[16]

4-fluoronitrobenzene (*o*-2k). ^{19}F NMR (282 MHz, THF) δ -76.56 (s, 1F).[17]

2-fluoronitrobenzene (*p*-2k). ^{19}F NMR (282 MHz, THF) δ -105.33 (M, 1F).[14]

2,3,5,6-tetrafluoropyridine (2m). ^{19}F NMR (282 MHz, THF) δ -93.26(s, 2F) , -141.47 (ddq, *J* = 30.3, 15.8, 8.2, 7.7 Hz, 2F).[14]

N,N-Dibenzylformamide (4a). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.43 (s, 1H), 7.55–7.05 (m, 10H), 4.42 (s, 2H), 4.27 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.8, 136.0, 135.7, 128.9, 128.7, 127.7, 50.3, 44.7.[18]

N-Formylpiperdine (4b). ^{1}H NMR (400 MHz, $CDCl_3$) δ7.80 (s, 1H), 3.44 – 3.18 (m, 2H), 3.20 – 3.07 (m, 2H), 1.49 (m, 2H), 1.44 – 1.24 (m, 4H).^{13}C NMR (101 MHz, $CDCl_3$) δ 160.7, 46.8, 40.5, 26.5, 25.0, 24.7.[19]

N-methyl-N-phenylformamide (4d). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.48 (s, 1H major rotamer), 8.36 (d, *J* = 2.5 Hz, 0.06H minor rotamer), 7.53 – 7.34 (t, *J* = 8.0Hz, 2.28H), 7.32 – 7.23 (t, *J* = 8.0 Hz, 1.08H), 7.17 (d, *J* = 8.0 Hz, 2.09H), 3.36 – 3.34 (s, 0.20H minor rotamer), 3.32 (s, 3H major rotamer).^{13}C NMR (101 MHz, $CDCl_3$) δ 162.3 (major rotamer), 162.2 (minor rotamer), 142.2 (major rotamer), 140.1 (minor rotamer), 129.6 (major rotamer), 129.0 (minor rotamer), 126.4 (major rotamer), 126.2 (minor rotamer), 123.6 (minor rotamer), 122.3 (major rotamer), 36.8 (minor rotamer), 32.0 (major rotamer). GC-MS (EI) (% relative intensity): m/z = 135 (100) $[M]^+$.[18]

***N*-Benzylformamide (4e).** ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.27 (s, 1H), 7.42 – 7.21 (m, 5H), 5.85 (s, 1H), 4.46 (dd, J = 28.1, 6.3 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.9, 137.5, 128.8, 127.8, 127.8, 127.0. GC-MS (EI) (% relative intensity): m/z = 135 (100) $[M]^+$.[20]

***N*-phenylformamide (4g).** ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.69 (d, *J* = 11.4 Hz, 1H), 8.39 (s, 1H), 7.66 (s, 1H), 7.54 (d, *J* = 7.9 Hz, 2H), 7.40-7.30 (m, 4H), 7.25 – 7.05 (m, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.8, 159.2, 136.9, 136.7, 129.8, 129.1, 125.3, 124.8, 120.0, 118.8.[21]

N-(4-bromophenyl)formamide (4h). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.65 (d, *J* = 11.5 Hz, 0.41H minor rotamer), 8.39 (s, 0.62H major rotamer), 7.46 (m, 4.25H), 6.96 (d, *J* = 7.4 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.2, 158.9, 135.9, 135.8, 132.8, 132.1, 121.5, 120.4, 117.5.[22]

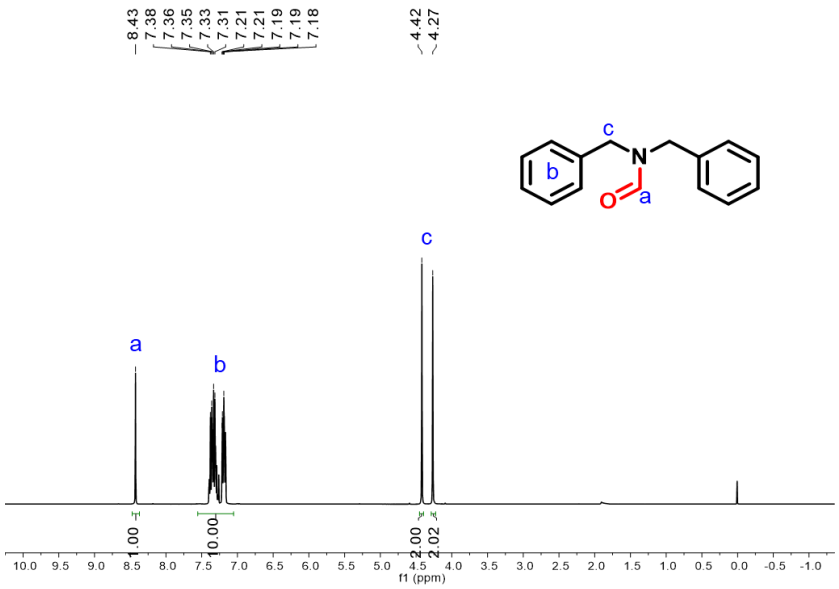


Figure S18. ^{1}H NMR (400 MHz, $CDCl_3$ solvent, 298 K) spectrum of **4a.**

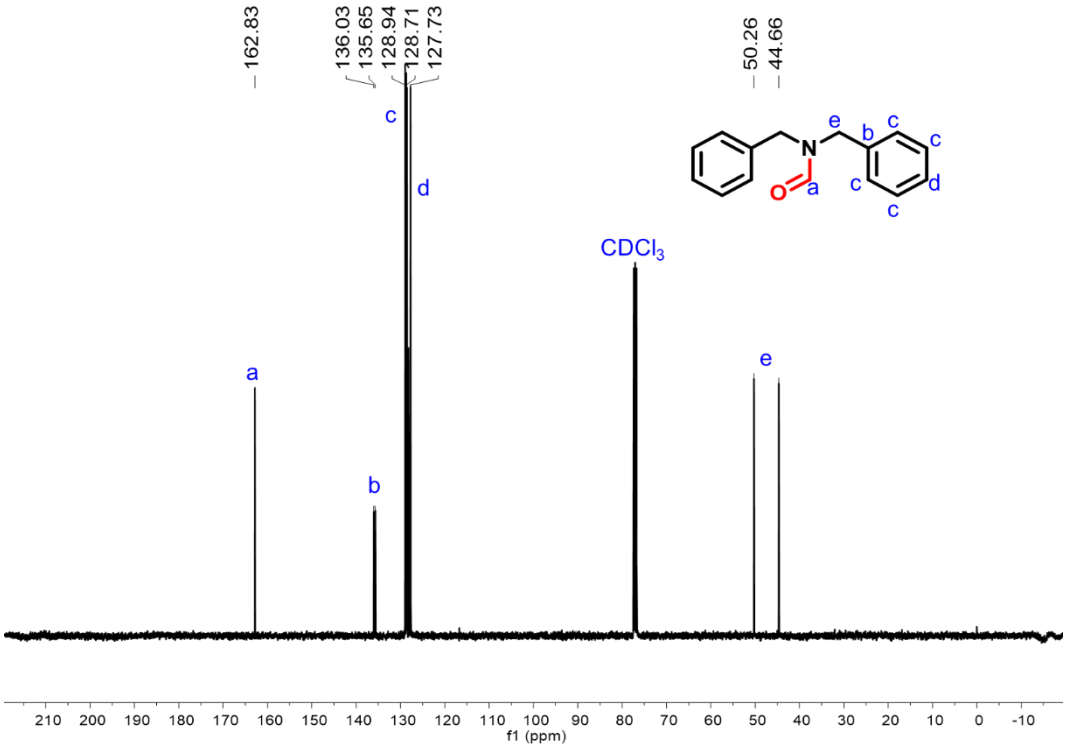


Figure S19. ^{13}C NMR (101 MHz, $CDCl_3$ solvent, 298 K) spectrum of **4a.**

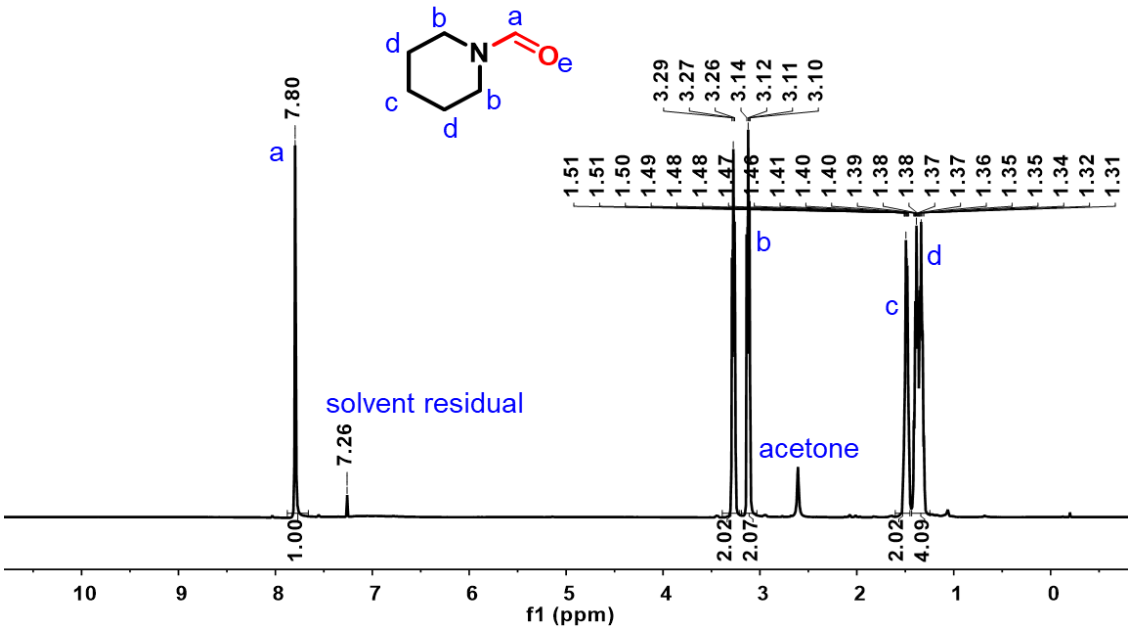


Figure S20. ^{1}H NMR (400 MHz, $CDCl_3$ solvent, 298 K) spectrum of **4b**.

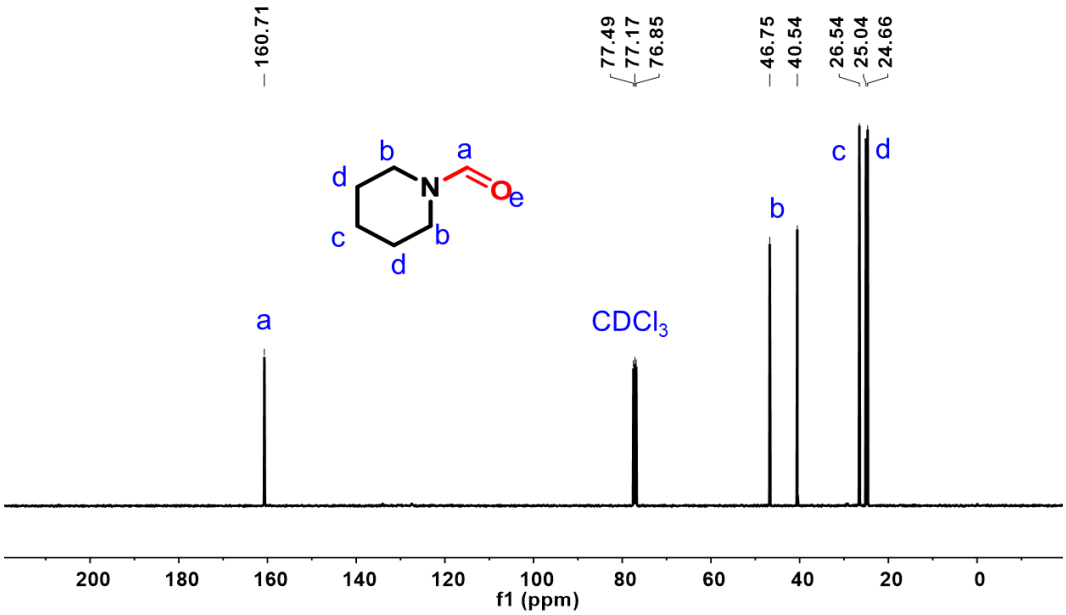


Figure S21. ^{13}C NMR (101 MHz, $CDCl_3$ solvent, 298 K) spectrum of **4b.**

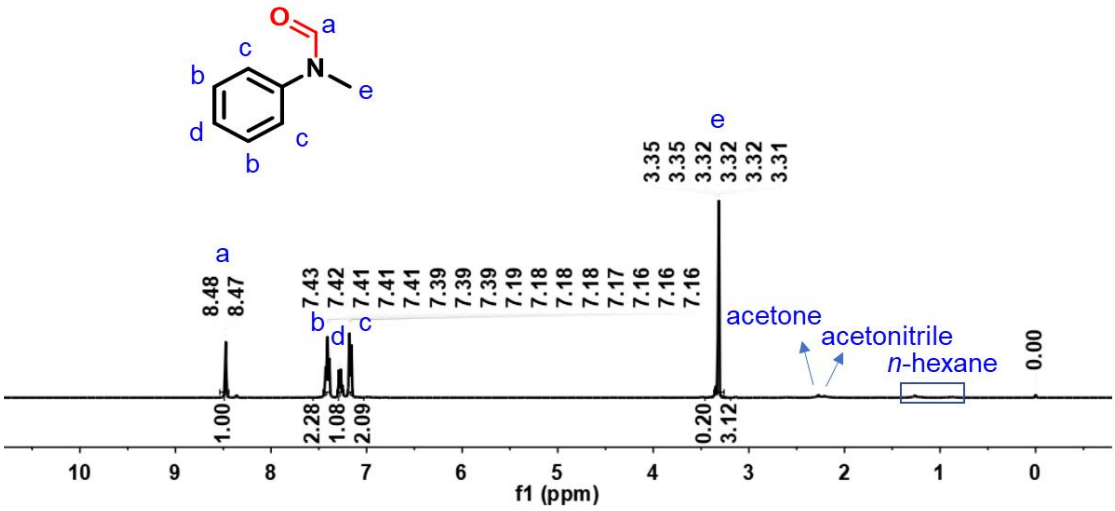


Figure S22. ^{1}H NMR (400 MHz, $CDCl_3$ solvent, 298 K) spectrum of **4d.**

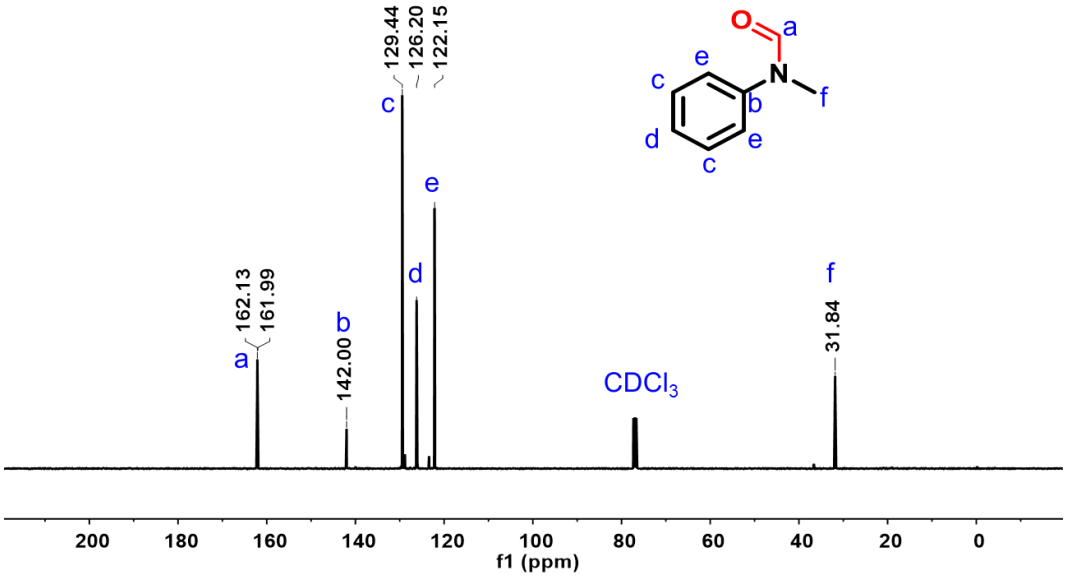


Figure S23. ^{13}C NMR (101 MHz, $CDCl_3$ solvent, 298 K) spectrum of **4d**.

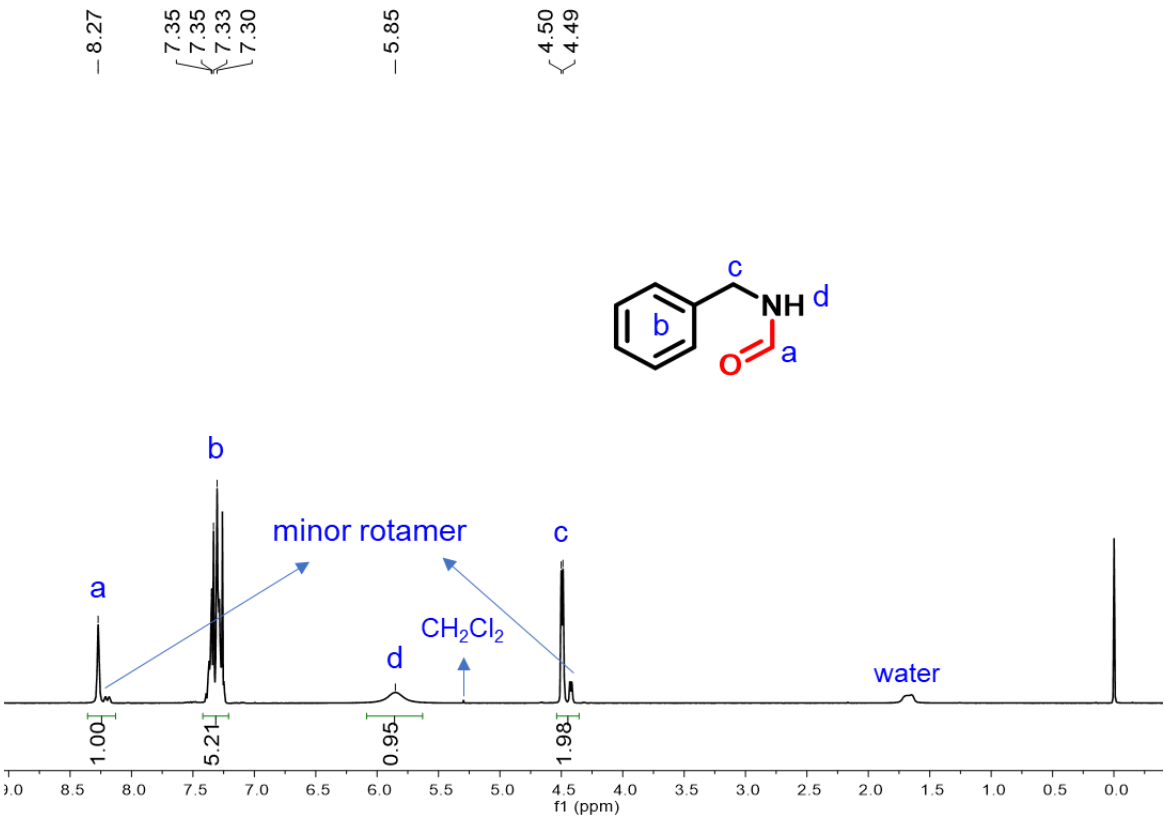


Figure S24. ^{1}H NMR (400 MHz, $CDCl_3$ solvent, 298 K) spectrum of **4e.**

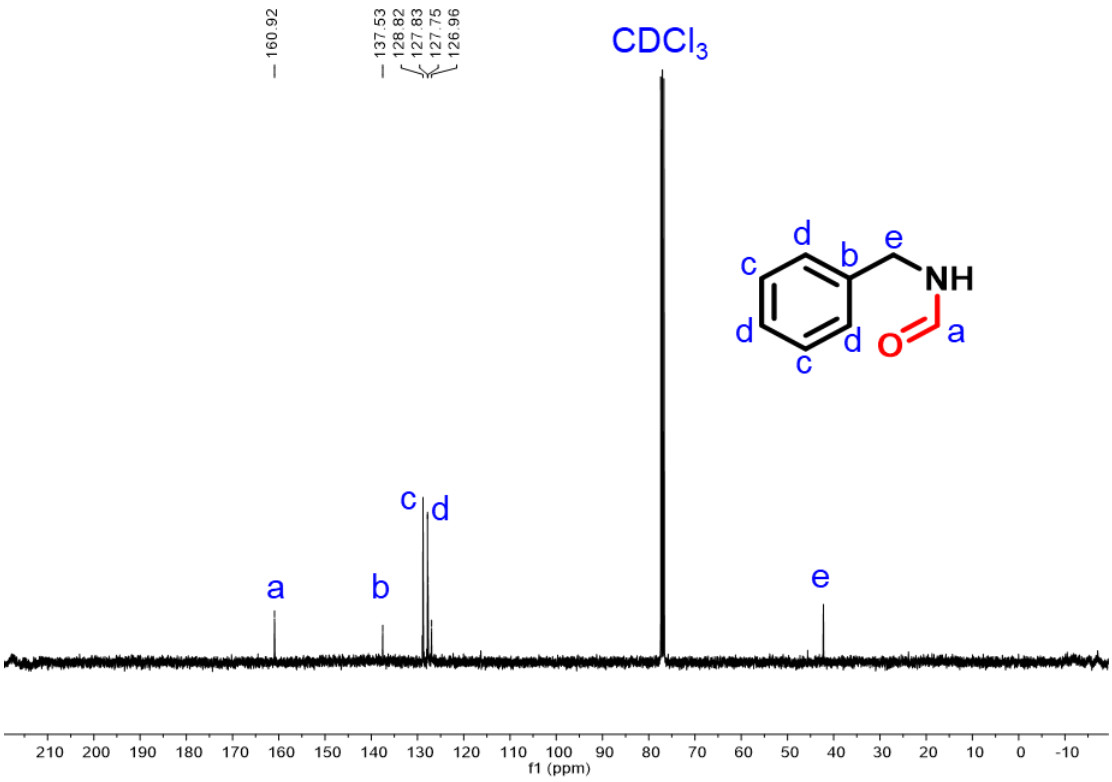


Figure S25. ^{13}C NMR (101 MHz, $CDCl_3$ solvent, 298 K) spectrum of **4e**.

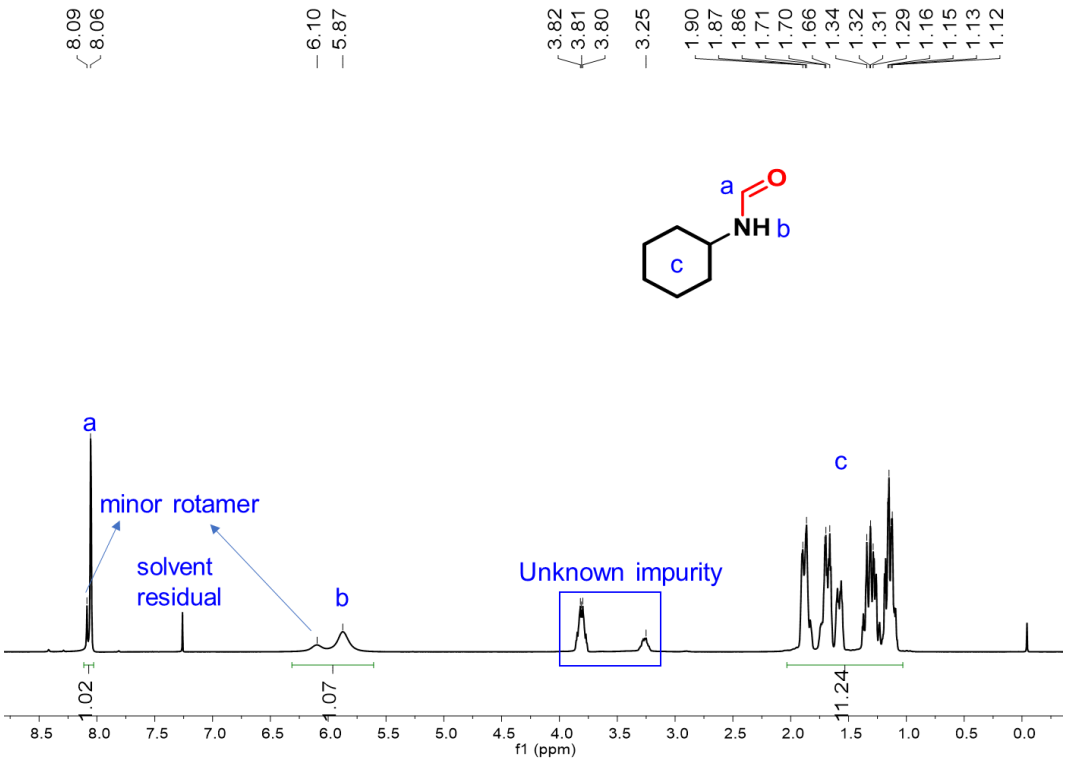


Figure S26. ^{1}H NMR (400 MHz, $CDCl_3$ solvent, 298 K) spectrum of **4f**.

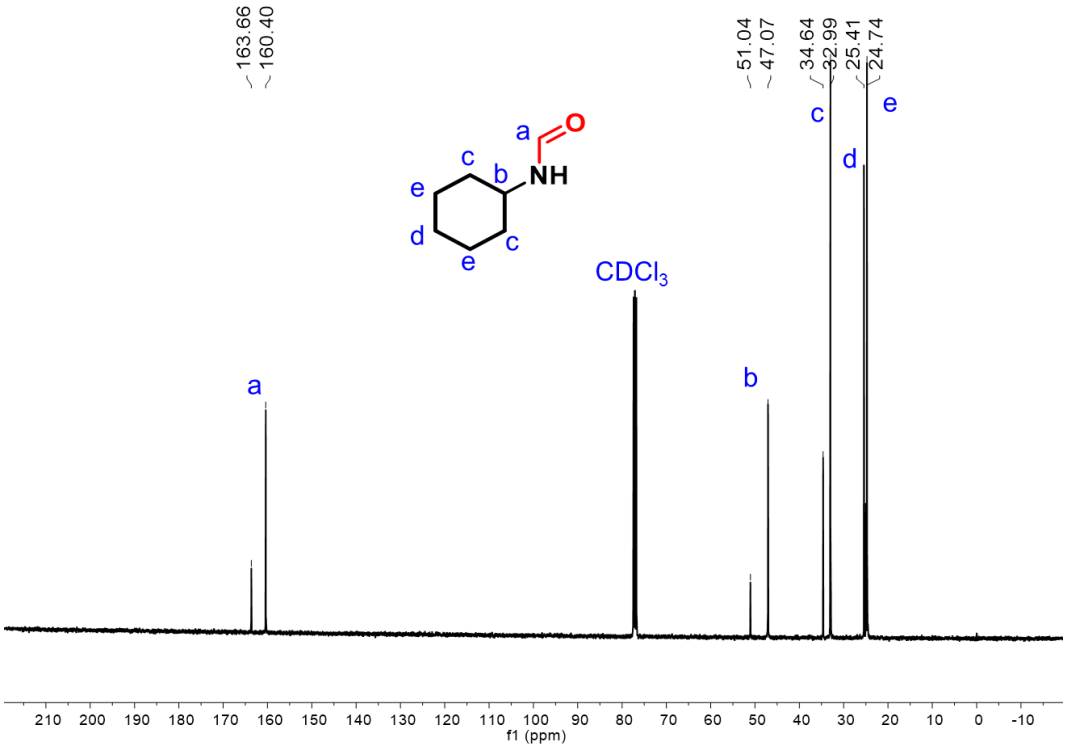


Figure S27. ^{13}C NMR (101 MHz, $CDCl_3$ solvent, 298 K) spectrum of **4f**.

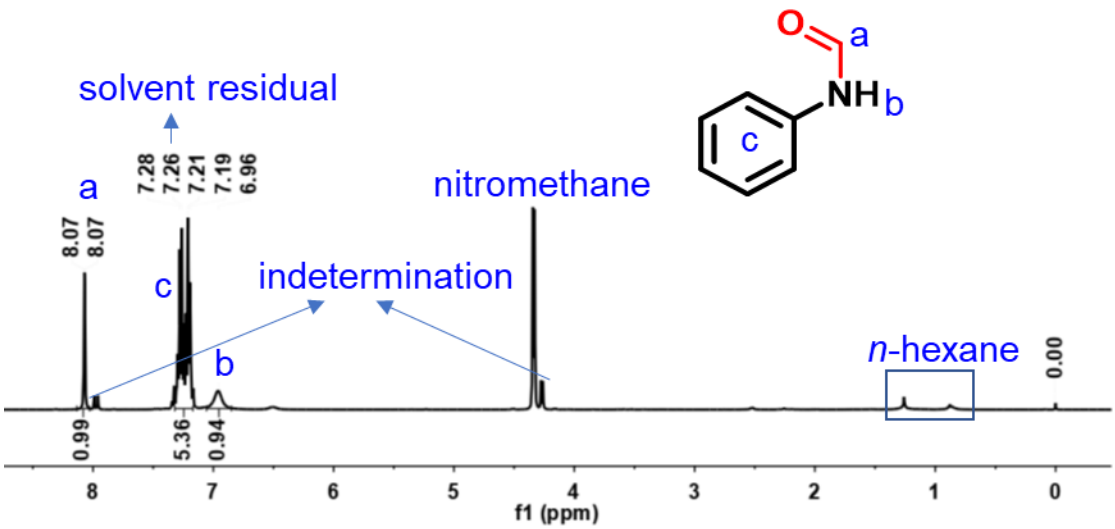


Figure S28. ^{1}H NMR (400 MHz, $CDCl_3$ solvent, 298 K) spectrum of **4g**.

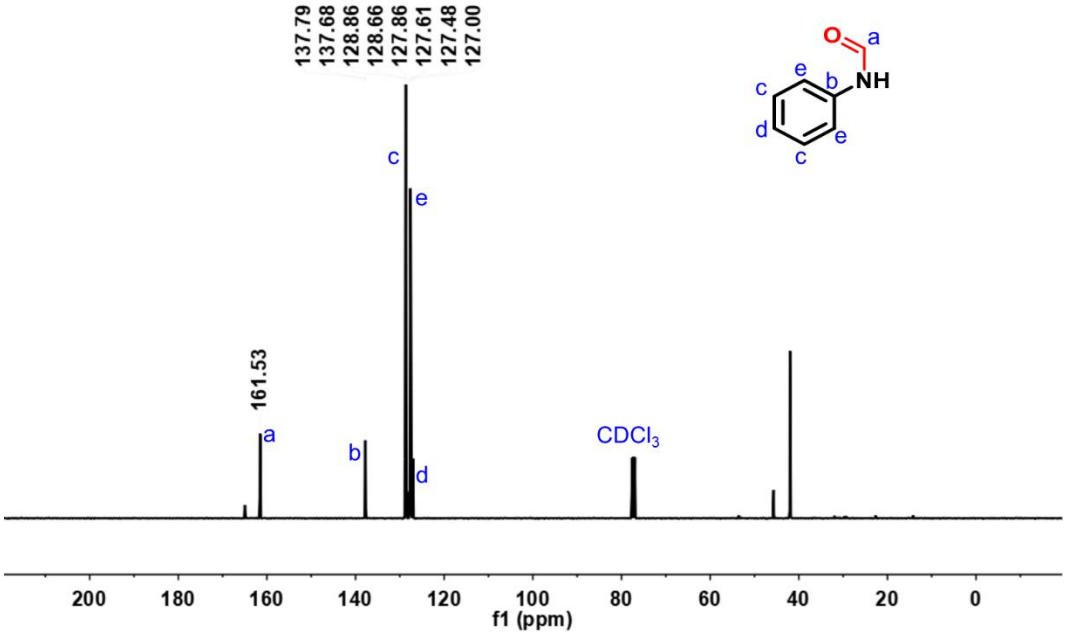


Figure S29. ^{13}C NMR (101 MHz, $CDCl_3$ solvent, 298 K) spectrum of **4g**.

9. Computed cartesian coordinates

[LAu-H] + CO_2

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H	2.83280200	-2.33125200	3.31045600

H	3.01854400	-2.80639700	1.60540200
H	1.43826200	-2.26240500	2.19850000
C	-2.44009700	-0.58885700	-2.53428600
H	-2.98380100	-0.82546700	-3.46456400
H	-1.42889300	-1.01185000	-2.61098900
H	-2.36812300	0.50786100	-2.46355600
C	4.78764100	0.06071000	-1.22141400
H	5.43288200	-0.36784900	-2.00721900
H	5.35580900	0.03888100	-0.28237700
H	4.59797300	1.10840200	-1.49291600
C	4.39278600	-0.43834700	2.20234700
H	4.61856200	-0.67613900	3.25582700
H	4.72390800	0.59392000	2.02882700
H	4.99781500	-1.11064900	1.57864000
C	-2.30613200	-0.60441600	2.95026800
H	-2.47026800	-1.12284700	3.90957500
H	-2.81984800	0.36560400	2.99799100
H	-1.22550300	-0.41571800	2.85149300
C	-4.35025600	-1.65635400	1.91733900
H	-4.58421300	-2.09043100	2.90420000
H	-4.74446300	-2.34384900	1.15651000
H	-4.89784000	-0.70757400	1.84543400
C	-4.63963400	-0.63861100	-1.34471500
H	-5.14225300	-0.97427200	-2.26787000
H	-4.65706400	0.46029700	-1.34648100
H	-5.23787900	-0.99557700	-0.49692400
C	2.71685100	-0.56490000	-2.47431900
H	3.38523600	-0.79728700	-3.32082700
H	2.37744400	0.47659300	-2.59706000
H	1.84351600	-1.23124400	-2.53048500
C	-3.22170400	-2.72007100	-1.46911000
H	-3.69257700	-2.99582000	-2.42795400
H	-3.80320700	-3.19720000	-0.66720400
H	-2.19938800	-3.12367400	-1.46962600
C	3.82208000	-2.24911500	-0.97360400
H	4.33093800	-2.61787300	-1.88040600
H	2.91850200	-2.85685100	-0.81921000
H	4.50309900	-2.41359300	-0.12552600
C	-0.56974900	4.20363200	-2.18321400
H	-0.48477600	3.16843100	-2.54509800
H	0.24008800	4.79382800	-2.63975700
H	-1.53535200	4.60828200	-2.52462800
C	-0.60439300	5.74096000	-0.20576500
H	-0.54130700	5.85419600	0.88722100

H	-1.56194100	6.16144000	-0.54355500
H	0.18614500	6.35106600	-0.66497100
H	0.65609400	-4.69304700	-2.42932500
C	0.56588600	-3.86129100	-1.66861500
O	0.90585300	-4.12140300	-0.50180300
O	0.12710100	-2.76970300	-2.12736800

INT1$_{CI}$

Charge = 0 Multiplicity = 1

C	3.39333900	-1.24230400	-0.11558700
C	2.57661500	-2.33760800	0.23369800
C	3.23491300	-3.52082600	0.61895800
H	2.65053900	-4.38982400	0.91028600
C	4.62407700	-3.60489600	0.66426100
H	5.10266800	-4.53528300	0.97761700
C	5.40284300	-2.50220900	0.30695900
H	6.48961300	-2.58075700	0.33556500
C	4.79833900	-1.31039700	-0.09776700
C	5.56597800	-0.08055000	-0.58465300
C	4.82470600	1.14798800	-0.05424600
C	5.45247600	2.31229100	0.39293300
H	6.54030700	2.36255300	0.43985100
C	4.69612500	3.42637600	0.76396400
H	5.19318900	4.33545300	1.10942300
C	3.30682300	3.38612100	0.67697400
H	2.73994600	4.27174600	0.95425400
C	2.62530800	2.23022500	0.25223500
C	3.41885700	1.11601800	-0.09074200
C	0.22955400	-2.78621300	2.02627900
C	0.19017800	-4.29708600	2.28514000
H	-0.07460400	-4.46350200	3.34311700
H	1.15589700	-4.78974200	2.11345900
H	-0.57368000	-4.79826200	1.67486500
C	-1.17132700	-2.20760500	2.28874700
H	-1.50070400	-2.50522800	3.29814000
H	-1.91812700	-2.57234600	1.57040500
H	-1.16069800	-1.11080000	2.24182400
C	1.22140300	-2.11093200	2.98817100
H	0.83588000	-2.19333100	4.01800600
H	1.34156500	-1.04030400	2.75897400
H	2.21459000	-2.57943900	2.95949800
C	0.18308300	-3.47404500	-1.08723700
C	0.77781100	-4.88579400	-1.00899700
H	0.33987200	-5.48838000	-1.82287900

H	0.55461900	-5.39891100	-0.06591100
H	1.86605900	-4.88311100	-1.16015900
C	-1.35119100	-3.53634000	-1.04116000
H	-1.71858900	-4.09236500	-1.91995300
H	-1.78971200	-2.53014900	-1.07935200
H	-1.71782800	-4.05606500	-0.14404900
C	0.63416500	-2.82652200	-2.40962700
H	0.34562800	-3.48620700	-3.24541800
H	1.72801800	-2.69970400	-2.44834800
H	0.15236200	-1.85096300	-2.56577700
C	0.44115600	3.33596700	-1.36728100
C	0.95236700	2.53495500	-2.57905800
H	0.78121100	3.12585100	-3.49476400
H	0.41625100	1.58106900	-2.68467800
H	2.03361200	2.33523300	-2.51060300
C	-1.07964500	3.51716600	-1.47797500
H	-1.31408400	4.01838000	-2.43236200
H	-1.48377100	4.14267600	-0.66934300
H	-1.59451300	2.54702700	-1.47686400
C	1.14439500	4.69835700	-1.34505200
H	0.84917800	5.25495800	-2.25084300
H	2.23832500	4.59777700	-1.36874500
H	0.86742800	5.31179000	-0.47893300
C	0.12091900	2.93494500	1.77392900
C	-1.32987300	2.43793900	1.90572200
H	-1.76848200	2.83820700	2.83473900
H	-1.36660300	1.34145700	1.95270600
H	-1.96351600	2.76025000	1.06957500
C	0.12490100	4.46370500	1.90216400
H	-0.25916200	4.73063800	2.90124500
H	-0.53265100	4.93967600	1.16212900
H	1.12661700	4.90412100	1.81366300
C	0.95755000	2.30779400	2.90084700
H	0.46484200	2.50602000	3.86731100
H	1.97382600	2.72271100	2.94739600
H	1.03929800	1.21579400	2.78369400
C	5.50637500	-0.05077000	-2.13479000
H	6.00134100	-0.94270500	-2.54963900
H	6.01976400	0.84566200	-2.51618500
H	4.46922400	-0.03340800	-2.50044200
C	7.03402300	-0.10415700	-0.15086500
H	7.13821300	-0.12791900	0.94456900
H	7.56367400	0.78072500	-0.53092700
H	7.54694900	-0.98220800	-0.56791200

O	2.81170900	-0.05255200	-0.48476800
P	0.72803000	-2.25251100	0.26046200
P	0.77919200	2.21965300	0.13187600
Au	0.02279700	-0.01913500	-0.18511300
H	-2.48983800	-0.16339500	0.60036900
Si	-3.91772900	-0.06485900	0.97559600
C	-4.58261600	1.61048100	0.42791000
C	-5.26876500	2.44965700	1.32518200
C	-4.36475000	2.07260000	-0.88471900
C	-5.72209100	3.71206200	0.92838800
H	-5.44671100	2.11929200	2.35300800
C	-4.81648600	3.33361800	-1.28345000
H	-3.80830600	1.44947200	-1.59104400
C	-5.49507100	4.15663300	-0.37787700
H	-6.25047700	4.35137500	1.64091200
H	-4.62907300	3.67908500	-2.30375100
H	-5.84479200	5.14464100	-0.68929700
C	-4.84989600	-1.52698100	0.23941300
C	-4.60911200	-1.93646100	-1.08724300
C	-5.79553000	-2.24307500	0.99716800
C	-5.29262700	-3.02627600	-1.63415000
H	-3.86699000	-1.40435900	-1.69052500
C	-6.48132100	-3.33288200	0.45109700
H	-5.99951000	-1.95108700	2.03187700
C	-6.22992900	-3.72653700	-0.86698600
H	-5.08883100	-3.33287200	-2.66376900
H	-7.21146300	-3.87740800	1.05605800
H	-6.76267000	-4.57987400	-1.29529300
H	-4.05872800	-0.13653600	2.46229600
Cl	-1.74291000	-0.02298700	-2.32202900

INT_F

Charge = 0 Multiplicity = 1

C	-2.98549700	1.16995600	-0.79893800
C	-2.42222700	2.27917000	-0.13704200
C	-3.20542000	3.44703600	-0.07962700
H	-2.81583500	4.32892800	0.42184200
C	-4.47891900	3.50411400	-0.63726600
H	-5.06468800	4.42266100	-0.56443400
C	-5.00073200	2.39112400	-1.29820100
H	-5.99280800	2.45040000	-1.74545700
C	-4.25680200	1.21499100	-1.39982600
C	-4.70370600	-0.02412100	-2.17598600
C	-4.26397200	-1.23831600	-1.35716500

C	-5.01526300	-2.40522300	-1.21292000
H	-6.01068900	-2.47201800	-1.65160100
C	-4.49600600	-3.50040800	-0.52082100
H	-5.08776100	-4.41174700	-0.41390300
C	-3.21559000	-3.43701500	0.01998800
H	-2.82535500	-4.30821500	0.53928300
C	-2.42441600	-2.27752700	-0.08019100
C	-2.98912000	-1.18263800	-0.76459100
C	-1.00126300	2.81458200	2.44522700
C	-1.13694200	4.32895300	2.65063200
H	-1.27818700	4.53042900	3.72598200
H	-2.00499300	4.75806900	2.13357600
H	-0.23777200	4.87513400	2.33581800
C	0.21499200	2.31696300	3.24978500
H	0.09404500	2.60587800	4.30711300
H	1.16122600	2.74358200	2.89195400
H	0.30858600	1.22207600	3.20459900
C	-2.26091200	2.10526600	2.96767000
H	-2.33205800	2.24013300	4.05967300
H	-2.22541400	1.02429600	2.76593200
H	-3.18124400	2.50176800	2.51739600
C	0.28681000	3.42304700	-0.39600900
C	-0.36515700	4.77680800	-0.70382300
H	0.35769900	5.38571400	-1.27230200
H	-0.62895500	5.34824000	0.19593200
H	-1.26161400	4.67308300	-1.33020300
C	1.62325000	3.64075900	0.32676800
H	2.34284100	4.11086600	-0.36064400
H	2.07085600	2.69494800	0.65451300
H	1.51766000	4.30291400	1.19873500
C	0.51979700	2.67564700	-1.72190000
H	1.11872800	3.31443000	-2.39107100
H	-0.43251100	2.45969800	-2.23339900
H	1.06749300	1.73312400	-1.58578100
C	0.27039400	-3.41282300	-0.43339100
C	0.47034500	-2.66541700	-1.76531400
H	0.96527300	-3.34579100	-2.47818000
H	1.10633900	-1.77398900	-1.67387300
H	-0.49273500	-2.36935500	-2.21237200
C	1.62722500	-3.65137400	0.24244900
H	2.32035300	-4.11668200	-0.47494200
H	1.54627000	-4.32534700	1.10780700
H	2.09334000	-2.71396000	0.56764800
C	-0.40987800	-4.75658000	-0.72661900

H	0.28872400	-5.37590400	-1.31377500
H	-1.32086100	-4.63781800	-1.32906800
H	-0.65982200	-5.32502500	0.17877000
C	-0.90892800	-2.82557600	2.45498700
C	0.33896600	-2.33285100	3.21338600
H	0.26035500	-2.62939800	4.27257700
H	0.43139800	-1.23774300	3.17238200
H	1.27013000	-2.75629400	2.81497000
C	-1.03466900	-4.34141500	2.65774700
H	-1.12724900	-4.54813900	3.73735000
H	-0.15047900	-4.88554400	2.30043700
H	-1.92473200	-4.76951700	2.17874900
C	-2.14597700	-2.12145300	3.03496400
H	-2.17680200	-2.27448000	4.12645600
H	-3.08412500	-2.50755900	2.61318700
H	-2.11401500	-1.03731000	2.85114400
C	-3.94802000	-0.05039000	-3.53085400
H	-4.21181000	0.83360500	-4.13202500
H	-4.21655700	-0.95381100	-4.10020200
H	-2.85825300	-0.05056000	-3.38565300
C	-6.20911600	-0.02449800	-2.45320100
H	-6.80073300	-0.00564600	-1.52551000
H	-6.49923900	-0.91384200	-3.03034600
H	-6.49389100	0.84479600	-3.06264800
O	-2.28238800	-0.00865900	-0.86311600
P	-0.74946100	2.22206900	0.64752600
P	-0.72847800	-2.21739600	0.65327500
Au	0.17296700	0.00656900	0.67973200
H	2.04328600	-0.00093600	0.75032500
Si	3.43448700	0.00129400	-0.06829800
C	4.24596600	-1.64639300	-0.60515400
C	4.98506400	-2.39836400	0.32378100
C	4.11620800	-2.16968800	-1.90560900
C	5.55143300	-3.63085700	-0.01479500
H	5.10490100	-2.00727700	1.33849700
C	4.69048200	-3.39337100	-2.25844800
H	3.53943800	-1.60726600	-2.64099600
C	5.40422000	-4.13335500	-1.31036100
H	6.11053000	-4.20127300	0.73257300
H	4.57551500	-3.77766300	-3.27626000
H	5.84545300	-5.09660800	-1.58129200
C	4.23598500	1.65796500	-0.59028900
C	4.09676500	2.19520400	-1.88389600
C	4.97730500	2.40243000	0.34295000

C	4.66380700	3.42535400	-2.22609300
H	3.51804400	1.63840200	-2.62194000
C	5.53686200	3.64089700	0.01510700
H	5.10427700	2.00062600	1.35257700
C	5.37991600	4.15755900	-1.27377500
H	4.54138100	3.82066600	-3.23881300
H	6.09799100	4.20506700	0.76567500
H	5.81560000	5.12565600	-1.53628600
F	2.37154900	0.00208300	-1.49286400
H	4.08696000	-0.00413800	1.33552500

[LAu-H] + Ph_2SiHF

Charge = 0 Multiplicity = 1

C	6.45055900	0.89058500	1.19888300
C	6.13548200	2.06515400	0.49049600
C	7.07436300	3.11204600	0.55043600
H	6.87954100	4.03869200	0.01681600
C	8.26077900	2.99046900	1.26981400
H	8.97427000	3.81746000	1.28640400
C	8.53054500	1.81856400	1.98111000
H	9.45179800	1.74091600	2.55876300
C	7.62305100	0.75760900	1.96589500
C	7.78635500	-0.52794300	2.77702300
C	7.29418000	-1.66950400	1.88726400
C	7.88695300	-2.93218800	1.82766100
H	8.78623100	-3.14182800	2.40694100
C	7.32837100	-3.93943600	1.03712300
H	7.79662000	-4.92543700	0.99524900
C	6.16725900	-3.69131100	0.30912400
H	5.74756800	-4.49397500	-0.29151900
C	5.53922400	-2.43141000	0.32467600
C	6.13905400	-1.43527600	1.11786500
C	5.04210700	2.92523100	-2.16469400
C	5.32471100	4.43164600	-2.23571000
H	5.59232500	4.69202700	-3.27433600
H	6.16316300	4.74551000	-1.60076400
H	4.44286400	5.02927500	-1.96700800
C	3.87742100	2.60610200	-3.12147200
H	4.13658400	2.95760400	-4.13457600
H	2.94370600	3.10056700	-2.82087400
H	3.68070900	1.52485100	-3.17166000
C	6.27877200	2.13769700	-2.62824100
H	6.46565800	2.34873300	-3.69460800
H	6.12812400	1.05191900	-2.52378300

H	7.18260100	2.41064600	-2.06629100
C	3.58127200	3.47252600	0.60341400
C	4.36307200	4.70986100	1.06173500
H	3.68360400	5.36094700	1.63843000
H	4.75314500	5.30321400	0.22507700
H	5.19953800	4.44773900	1.72378800
C	2.33177200	3.90926200	-0.17514200
H	1.67025300	4.48374000	0.49521600
H	1.76882900	3.04239400	-0.54982800
H	2.58375900	4.55846300	-1.02635200
C	3.15277600	2.67613000	1.84963000
H	2.55801900	3.32637500	2.51329400
H	4.02275900	2.31967200	2.42410300
H	2.53685800	1.80462500	1.57923700
C	2.70734500	-3.16953600	0.22055400
C	2.42718600	-2.43795500	1.54622300
H	1.66043200	-2.99089500	2.11491000
H	2.05676400	-1.41590900	1.37328400
H	3.32965300	-2.37677100	2.17551200
C	1.42906300	-3.18744500	-0.63061700
H	0.61116800	-3.63923400	-0.04410200
H	1.55101400	-3.78862700	-1.54332700
H	1.12152000	-2.17186800	-0.91795600
C	3.13060500	-4.60867700	0.54019200
H	2.27681400	-5.13021900	1.00622600
H	3.96177300	-4.64493500	1.25742500
H	3.41494300	-5.17953200	-0.35303000
C	4.40129100	-2.69115900	-2.42809700
C	3.38586200	-2.00779900	-3.36331700
H	3.60962600	-2.28872900	-4.40640600
H	3.43728400	-0.91164900	-3.28327500
H	2.35183500	-2.30900900	-3.14699500
C	4.34350100	-4.20442700	-2.67273600
H	4.58711800	-4.40065600	-3.73125600
H	3.34177400	-4.61566400	-2.48785800
H	5.06775100	-4.76627800	-2.06902600
C	5.80492100	-2.16131600	-2.76507700
H	5.99316400	-2.28843200	-3.84445900
H	6.59412000	-2.69624700	-2.21869200
H	5.89724000	-1.08884300	-2.53289100
C	6.86340700	-0.44236400	4.02080800
H	7.16908900	0.39853600	4.66287600
H	6.92843100	-1.37300100	4.60607000
H	5.81231000	-0.29041400	3.73480600

C	9.22760400	-0.73721900	3.24877600
H	9.92997800	-0.80600000	2.40423700
H	9.31103700	-1.65653700	3.84551500
H	9.54578400	0.09072400	3.89797200
O	5.58659500	-0.17665700	1.13549600
P	4.55145200	2.21243200	-0.45842500
P	4.00863600	-2.07846800	-0.65877200
Au	3.08089600	0.23344900	-0.75213100
H	1.40846100	0.43523700	-0.93514100
Si	-14.43505300	-0.00388300	0.58965700
C	-15.46969400	-1.52429300	0.28805000
C	-14.88553500	-2.69902600	-0.22262900
C	-16.84949200	-1.52902900	0.57233100
C	-15.65417200	-3.84594100	-0.43909200
H	-13.81709800	-2.72017800	-0.45710500
C	-17.61934300	-2.67470500	0.35915200
H	-17.32971600	-0.62650600	0.96065700
C	-17.02165800	-3.83397900	-0.14731200
H	-15.18672900	-4.74986300	-0.83781300
H	-18.68874000	-2.66388400	0.58474100
H	-17.62449200	-4.72976300	-0.31775000
C	-15.38792000	1.57066700	0.27746000
C	-15.31707700	2.64534100	1.18312400
C	-16.18276100	1.71485800	-0.87588400
C	-16.01774700	3.83057900	0.94237500
H	-14.71225700	2.55307500	2.08895200
C	-16.88115700	2.89997500	-1.11990000
H	-16.26534300	0.89091300	-1.59104300
C	-16.79888800	3.95956400	-0.21006500
H	-15.95501200	4.65548800	1.65681200
H	-17.49439800	2.99648500	-2.01951000
H	-17.34689500	4.88630800	-0.39905800
F	-13.97144800	0.05934700	2.17090800
H	-13.16854100	-0.10121200	-0.18332200

TS2

Charge = 0 Multiplicity = 1

Au	-0.44204100	-0.03606900	0.37049500
P	0.63660500	2.22680700	0.35505000
P	0.74982800	-2.23106300	0.33718600
C	2.59003900	-2.23384400	0.04000300
C	3.16922100	3.54392000	0.16116400
H	2.64819800	4.41808000	0.52495800
C	3.26544800	-1.10977600	-0.47494700

C	3.19466200	1.25002900	-0.51923600
C	2.45724800	2.34494500	-0.02795100
C	3.37598200	-3.37505200	0.28564400
H	2.90848700	-4.27072400	0.66980000
C	4.74620400	-3.39370900	0.04961200
H	5.32170400	-4.28856500	0.26574100
C	4.63880200	-1.12017800	-0.77736400
C	4.56226300	1.33548200	-0.83525200
C	4.53058200	3.64418500	-0.10325400
H	5.04911500	4.58265200	0.06731200
C	5.22022500	0.11146300	-1.47462400
C	5.37224600	-2.27070000	-0.48751700
H	6.43598500	-2.30232800	-0.69311500
C	5.22190200	2.54247800	-0.60317600
H	6.27926200	2.63425700	-0.82344900
O	2.54364700	0.04542300	-0.71294700
C	0.11744100	-3.25420000	-1.16677000
C	0.41994400	3.04429400	2.09289800
C	0.48019100	-3.13694600	2.02356600
C	-0.14137100	3.26763500	-1.06661700
C	-0.94502100	2.57391100	2.64387500
H	-1.07061000	2.97024300	3.65939400
H	-1.01131800	1.48406700	2.69453700
H	-1.78693200	2.92211100	2.04413000
C	1.50575600	-2.55551300	3.02041800
H	1.26403100	-2.91463400	4.02782600
H	1.46780100	-1.46118700	3.04298400
H	2.53156400	-2.85519500	2.79398900
C	-0.93359100	-2.75515200	2.51722400
H	-1.09864600	-3.21464200	3.49999700
H	-1.72404600	-3.10285800	1.85065600
H	-1.05250100	-1.67452700	2.62462500
C	-0.02235200	2.37871700	-2.32504300
H	-0.46156700	2.90625700	-3.18032600
H	-0.55766400	1.43274300	-2.19998000
H	1.02057600	2.15545200	-2.57244900
C	0.89226400	-4.55325200	-1.45715500
H	0.44118500	-5.03877300	-2.33125000
H	0.84575700	-5.26699500	-0.63156400
H	1.94212900	-4.36545700	-1.69329400
C	0.57316700	-4.67620900	2.02351500
H	0.37963200	-5.03432700	3.04221700
H	1.55425600	-5.05918900	1.73635800
H	-0.17735300	-5.13457600	1.37556200

C	1.52724300	2.46621400	2.99970600
H	1.33113300	2.76634800	4.03599500
H	2.52254300	2.82505900	2.72751500
H	1.53965200	1.37135000	2.96825400
C	0.44806400	4.58387500	2.15970500
H	0.28004800	4.88906100	3.19996600
H	-0.34430800	5.03821100	1.56064600
H	1.40289700	5.01757400	1.85650000
C	0.53629500	4.61895900	-1.36104500
H	-0.00414900	5.10652300	-2.18171600
H	1.57422100	4.50008000	-1.67973100
H	0.51165000	5.30209500	-0.50869300
C	0.26362500	-2.31456700	-2.38434900
H	-0.09918800	-2.83082800	-3.28134800
H	1.30626400	-2.03262400	-2.56186900
H	-0.32359800	-1.40009200	-2.25849700
C	-1.63214600	3.49824400	-0.76249600
H	-2.11728500	3.91937000	-1.65129400
H	-1.78601600	4.20597700	0.05687600
H	-2.14286300	2.56983700	-0.50684600
C	-1.37364100	-3.58029600	-0.96993600
H	-1.77293400	-3.99708500	-1.90252600
H	-1.95770000	-2.69474500	-0.71885500
H	-1.53715500	-4.32573900	-0.18668500
C	4.81710800	0.06226900	-2.97784000
H	3.73144600	0.02793900	-3.09895400
H	5.24232800	-0.82685000	-3.45473600
H	5.19085700	0.94954000	-3.49921900
C	6.75411100	0.16145500	-1.38614300
H	7.10405400	0.19902100	-0.35002100
H	7.14264600	1.03580900	-1.91462200
H	7.19728900	-0.71293400	-1.86961000
H	-2.20548600	-0.05876500	0.31047700
C	-5.21478400	1.17508100	-0.63308700
C	-5.66207500	0.01564100	-1.30113900
C	-5.17704000	-1.21828100	-0.81794500
C	-4.32635500	-1.28747100	0.26123400
C	-3.75088100	-0.11922400	0.83167500
C	-4.36360600	1.10417700	0.44570700
F	-3.94910000	2.23926700	1.04796400
F	-3.34663300	-0.21231100	2.13802000
F	-3.87321700	-2.48788700	0.68174800
F	-5.58061500	-2.35414000	-1.40377900
F	-5.65497600	2.37467900	-1.03767200

C	-6.55585800	0.08648700	-2.39930300
N	-7.28669200	0.14526200	-3.30482900

TS for $[Ph_2SiH_2F]^-$ catalyzed HDF reaction

Charge = 0 Multiplicity = 1

H	-0.04199800	-1.55811100	-1.09712800
Si	-1.50815300	-0.88292900	-0.73748700
H	-1.89314600	-1.16914400	-2.18254200
C	-3.31128600	-0.31257400	-0.23782500
C	-3.95014000	-0.63117600	0.97484000
C	-4.01146600	0.52650000	-1.12512800
C	-5.22102500	-0.13343200	1.29076500
H	-3.43988700	-1.28587300	1.68558500
C	-5.27867200	1.03389800	-0.82272500
H	-3.55021700	0.79376500	-2.08370200
C	-5.88995000	0.70384200	0.39284700
H	-5.69158800	-0.40034100	2.24214600
H	-5.79396600	1.68637800	-1.53422200
H	-6.88179100	1.09538100	0.63611400
C	-0.61033700	0.77770400	-0.51417100
C	-0.60811700	1.42227600	0.73632400
C	0.11889300	1.37047300	-1.56043300
C	0.10379100	2.60765200	0.93867300
H	-1.16840400	0.98694300	1.56962700
C	0.80624000	2.57416900	-1.37564600
H	0.16757900	0.87369400	-2.53480500
C	0.81019700	3.18925900	-0.12009500
H	0.11277900	3.08005200	1.92483500
H	1.36407900	3.01835000	-2.20421400
H	1.37270600	4.11281600	0.03849500
F	-1.43153800	-1.93714100	0.58808500
C	1.61908800	-1.91967800	-0.53440400
C	2.36362400	-0.98393300	-1.28751100
C	1.61556600	-1.76344000	0.87113500
C	2.89392400	0.14388100	-0.69625000
C	2.12879700	-0.62030600	1.45230900
C	2.81450100	0.35233300	0.69555000
F	1.46264500	-3.16115400	-1.03019600
F	1.02705100	-2.69389000	1.62560100
F	2.02255400	-0.45878700	2.77206200
F	3.51118000	1.04861400	-1.45704500
F	2.40338100	-1.12633000	-2.61814100
C	3.37965000	1.49987800	1.30481100
N	3.85155500	2.43733300	1.80613400

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